SUPREM-III User's Manual

Version 8520

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Introduction

SUPREM-III is a computer program that allows the user to simulate the various processing steps used in the manufacture of silicon integrated circuits or discrete devices. The types of processing steps simulated by the current version of the program are: inert ambient drive-in; oxidation of silicon and silicon-nitride; ion implantation, epitaxial growth of silicon; and low temperature deposition or etching of various materials. SUPREM-III simulates in one dimension the changes in a semiconductor structure as a result of the various processing steps used in its manufacture. The primary results of interest are the thicknesses of the various layers of materials that make up the structure and the distribution of impurities within those layers. The program will also determine certain material properties such as polysilicon grain size and the sheet resistivity of diffused regions in silicon layers.

I. The Simulation Structure

In SUPREM-III, a structure whose processing is being simulated is made up of from one to ten layers, each of which is composed of one of ten possible materials. The same material may appear in more than one layer. The default materials defined in SUPREM-III are single crystal silicon, poly-crystalline silicon, silicon dioxide, silicon nitride, and aluminum. The layers in a structure are numbered sequentially, the bottommost layer being layer one. Diffused regions within a layer are also numbered sequentially with the bottommost region in each layer being region one of that layer. A SUPREM-III structure may be doped with up to four impurities, with the default impurities being boron, phosphorus, arsenic, and antimony.

II. Using SUPREM-III

To begin a SUPREM-III simulation, all of the coefficients and parameters for the materials and impurities must be input and the initial structure defined. Both of these functions are accomplished by the INITIALIZE statement. In its simplest form the initial structure is a single layer of substrate material, though a more complicated multi-layer structure generated by a previous simulation may be specified. The coefficients are normally read from the default coefficient file and the structure may either be read from a previously saved structure file or defined through the parameters of the INITIALIZE statement. In the data file containing the input statements that control the SUPREM-III simulation, the INITIALIZE statement must precede all other statements except TITLE, COMMENT, or STOP statements.

Once the coefficients and the initial structure have been defined, process simulation can begin. If the user wishes to change any of the material or impurity coefficients, new values may be input by usingthe model parameter statements. The coefficients defining the impurities are accessed through the impurity statements, BORON, PHOSPHORUS, ARSEN-IC, ANTIMONY, and IMPURITY. The material coefficients are accessed through the SILICON, POLYSILICON, OXIDE, NITRIDE, ALUMINUM, and MATERIAL statements. Other coefficients that apply to the interaction of materials and impurities may be controlled through the SEGREGATION, VOL.RATIO, and MOBILITY statements. Oxidation rates are controlled by the parameters of the DRYO2, WETO2, and NITROGEN statements. If a user alters any of the coefficients, by using the SAVEFILE statement he may save the modified set of coefficients either into the default coefficient file, S3cof0, creating a new set of defaults, or into an alternate coefficient file that can be read in with either the INITIALIZE or the LOADFILE statements.

III. The SUPREM-III Grid Structure

In SUPREM-III, the structure is made up of a series of cells. These cells are laid out on a one-dimensional grid of points called nodes. Within each layer, each cell is centered about a single node point. The cells at either end of a layer are half-cells, with one cell boundary at the endpoint node and the other halfway to the adjacent node within the layer. Within each cell, the physical coefficients and any impurity

concentrations are treated as constant. In the current version of the program there may be a maximum of 500 node points or 499 cells or spaces. If an attempt is made to use more than the maximum number of node points during a simulation, the program will terminate with an error.

The distance between adjacent node points within each layer can be controlled by the user, either when a layer is first defined in an INITIALIZE or DEPOSITION statement or at any time in the simulation through the GRID statement. The grid placement is controlled by five parameters; the layer thickness (THICKNESS), the nominal grid spacing (DX), the location of the nominal grid spacing relative to the top surface of the layer (XDX), the number of spaces in the layer (SPACES), and the minimum allowed grid spacing (DX.MIN). The way these parameters are used to control the grid spacing is described below. For the purposes of example, assume that a layer is being deposited on the structure.

In the simplest case the user need only specify the layer's thickness. In this case the program will assume that XDX is zero, placing the nominal grid spacing, DX, at the surface of the layer and will use the default DX for the deposited material. The deposited material, specified by name, has its characteristics, including its default DX, defined by the appropriate material statement. The program will use the number of spaces necessary to achieve a uniform grid spacing throughout the layer.

If the default DX is not adequate, then the user may specify both the thickness and the DX, and the program will work as above except that the specified DX will be used instead of the default value.

In many cases, both to save execution time and to have the structure fit within the limit of 499 grid spaces, a fewer number of spaces may be specified than the program would allocate for uniform grid spacing within the layer. In this case a non-uniform grid spacing will be set up within the affected layer. If the number of spaces specified is less than the number needed for a uniform grid spacing, the program will place a grid spacing of DX at the location specified by XDX, and cause the grid spacings to increase parabolically to either side (figure 1). If the number of spaces specified is greater than the number needed for uniform grid spacings, then the grid spacings will decrease from the DX value on either side of XDX (figure 2).

```
     |                      |                          |                       |
     |          *           | dX2                 dX |          *            |
dX1 |     *    *             |                          |      *         *       |
     |    *          *       |                     dX1 |         *      *        |
dX   |       *               |                          |          *           |  dX2
     |_______________________|                          |_______________________|
     0                   XdX  thickness                0Xd                    Xthickness
figure 1                                           figure 2
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When a non-uniform grid is set up, the program first determines what the maximum grid spacing would be at either end of the layer assuming a linear variation in grid spacing from XDX, given DX, XDX, the layer thickness and the number of spaces to use. Then with the nominal DX and the two endpoint grid spacings, the grid is made to vary parabolically from DX to the endpoints in such a way that the resulting grid gives a layer of the specified thickness. With this algorithm the user can minimize the number of grid spacings used in the solution and yet place a fine mesh where it is needed to accurately represent a rapidly varying impurity distribution.

IV. SUPREM-III Output

The results of a SUPREM-III simulation are available in both printed and graphic forms. Printed output can consist of the following: all material and impurity coefficients as might have been specified by one or more of the MATERIAL, IMPURITY, SEGREGATION, or VOL.RATIO statements; information about the current structure such as the thicknesses and com-position of the various layers, impurity junction depths, or resistivity of layers or diffused regions; and the impurity concentrations at each node

point and the distance of that point from the structure surface. Plotted or graphic output consists of plots of the specified impurity concentrations versus distance.

V. SUPREM-III Input Statements

SUPREM-III normally takes its input from a user specified disk file. This file is madeup of various statements identified by a statement name followed by a parameter list. The statement name is delimited from the parameter list by either a comma and/or one or more blanks. If a comma is present, it may be preceded or followed by any number of blanks. Parameters in a SUPREM-III parameter list are delimited from each other in the same way the statement name is delimited. If more than one line of input is required for a particular statement, it may be continued on subsequent lines by placing a plus sign as the first non-blank character on the continuation lines.

Parameters in a SUPREM-III parameter list may be one of three types that correspond to the types of values that they may take on. These types are; Logical, numerical, and character. Logical parameters take on a value of true if the parameter name appears by itself and a value of false if it is preceded by the NOT, (^), character. Numerical type parameters are assigned values in the parameter list by having the parameter name followed by an equal sign and the value. Blanks on either side of the equal sign are ignored. Character parameters may appear in one of two ways depending of the statement involved. In one case they have a formal parameter name and they are assigned a character string by use of an equal sign in the same way as a numerical parameter. In the other case the statement has the character parameter as the only valid parameter and the character string appears by itself following the statement name without an associated parameter name.

VI. Manual Format

This manual presents each statement showing the statement name and the associated list of parameters. There are a number of special characters that are used to aid in the description of the parameter lists. These characters are <, >, [,], (,), and |.

The <> characters are used to indicate classes of things. For example a parameter description might appear as:

CONCENTRATION=<n>

which indicates that the parameter name is concentration and it is assigned a numerical value. The <n> defines a class of things represented by n, where n represents the set of numerical values. Valid numerical values are of the form:

9 1.2 -.345 6.7E8 -9.01E-2

The only other class defined in this manual is that of character strings represented by <c>.

The [] characters enclose sets of optional items, usually parameters. For example:

STMT1 [PARM1] [PARM2 PARM3] [PARM4 [PARM5]]

indicates that on the STMT1 statement, the PARM1 parameter is optional. PARM2 and PARM3 are optional but if one is specified, both must be specified. PARM4 and PARM5 are optional but PARM5 may be specified only if PARM4 is specified.

When one or more of a list of items are to be chosen from, they are separated by a | character and enclosed in parenthesis. For example:

STMT2 (PARM1 | PARM2 | (PARM3 PARM4))

This indicates that statement STMT2 requires that either PARM1, PARM2, or both PARM3 and PARM4 be specified. In none of the above examples are the special characters actually typed by the user when inputting a SUPREM-III input sequence.

VII. Aluminum Statement

The ALUMINUM statement is used to input or modify the characteristics of aluminum as a layer material.

ALUMINUM
[NAME=<c>] [DX.DEFAU=<n>] [CONDUCTO] [SPECIES=<n>] [DENSITY=<n>][AT.WT.1=<n>] [AT.NUM.1=<n>] [ABUND.1=<n>] [WORK.FUN=<n>] [EPSILONF=<n>]

Name	Type	Description	Unit	Default
ABUND.1	Num	The relative abundance of element one in the material. The sum of all abundances for a material must equal one.		the current value
AT.NUM.1	Num	The atomic number of element one in the material.		the current value
AT.WT.1	Num	The atomic weight of element one in the material.	amu	the current value
CONDUCTO	Log	Specifies that the material is a conductor.		false
DENSITY	Num	The density of the material.	grams/cm^3	the current value
DX.DEFAU	Num	The default nominal grid spacing for any layer containing this material.	μm	the current value
EPSILONF	Num	The dielectric constant of the material relative the dielectric constant of air.		the current value
NAME	Char	The name of the material.		the current name of the material
SPECIES	Num	The number of different elements in this material.		the current value
WORK.FUN	Num	The work function of the material.	volts	the current value

The ALUMINUM statement is an alias for the MATERIAL statement with an index of five and is used to define or modify the parameters and coefficients associated with the material aluminum. Not all of the parameters of the MATERIAL statement apply to aluminum and so are not listed here.

VIII. Antimony Statement

The ANTIMONY statement is used to input or modify the physical or model coefficients associated with antimony as a dopant impurity.

ANTIMONY
[NAME=<c>] [DONOR] [AT.WT=<n>] [AT.NUMB=<n>] [IONFILE1=<c>] [IONFILE2=<c>]
[((SILICON [FII.0=<n>] [FII.E=<n>] [K.MF=<n>] [K.A=<n>] [K.P=<n>]) | (POLYSILI [FII.0=<n>] [FII.E=<n>] [ENTROPY=<n>] [HEAT.SEG=<n>] [Q.SITES=<n>]) | (OXIDE | NITRIDE | ALUMINUM)
[ELECT.ST=<n>] [DIX.0=<n>] [DIX.E=<n>] [DIM.0=<n>] [DIM.E=<n>] [DIMM.0=<n>] [DIMM.E=<n>]]

Name	Type	Description	Unit	Default
ALUMINUM	Log	Specifies that the material dependent parameters apply to antimony in aluminum		false
AT.NUMB	Num	The atomic number of the impurity		the current value
AT.WT	Num	The atomic weight of the impurity	amu	the current value
DIM.0	Num	The pre-exponential constant of the diffusion coefficient of the impurity diffusing with singly negative vacancies	μm^2/min.	the current value
DIM.E	Num	The activation energy of the diffusion coefficient of the impurity diffusing with singly negative vacancies	eV	the current value
DIMM.0	Num	The pre-exponential constant of the diffusion coefficient of the impurity diffusing with doubly negative vacancies	$microns^2$/min.	the current value
DIMM.E	Num	The activation energy of the diffusion coefficient of the impurity diffusing with doubly negative vacancies.	eV	the current value
DIX.0	Num	The pre-exponential constant of the diffusion coefficient of the impurity diffusing with neutral vacancies.	μm^2/min.	the current value
DIX.E	Num	The activation energy of the diffusion coefficient of the impurity diffusing with neutral vacancies.	eV	the current value
DONOR	Log	Specifies that the impurity is a donor.		the current value
ELECT.ST	Num	The electric stopping power of the impurity in the specified material	(KeV/ µm.)	the current value
ENTROPY	Num	The entropy factor. Used to calculate the equilibrium segregation factor at polysilicon grain boundaries.		the current value
FII.0	Num	The pre-exponential constant of the fractional partial-interstitialcy contribution	$(\mu m/min)^{-1/2}$	the current value
FII.E	Num	The activation energy of the fractional partial interstitialcy contribution	eV	the current value
HEAT.SEG	Num	The activation energy of the equilibrium segregation factor at polysilicon grain boundaries	eV	the current value
IONFILE1	Char	Specifies the primary ion implant range data file for implants using the analytic distributions. This file will be searched for the range statistics when implanting atomic antimony		the last file specified
IONFILE2	Char	Specifies the secondary ion implant range data file for implants using the analytic distrbutions. This file will be searched for the range statistics when implanting the compound ions containing antimony.		the last file specified
K.A	Num	Used in R. Reif's epitaxial doping model (see reference in EPITAXY statement). K.a is a thermodynamic constant relating	cm	the current value

		the dopant species concentration in solid silicon and adsorbed layer		
K.MF	Num	Used in R. Reif's epitaxial doping model (see reference in EPITAXY statement). K.mf is a kinetic coefficient controlling the rate-limiting step of the dopant incorporation process	cm^{-2} min^{-1} atm^{-1}	the current value
K.P	Num	Used in R. Reif's epitaxial doping model (see reference in EPITAXY statement). K.p is a thermodynamic constant relating the dopant species concentration in solid silicon and gas phase	cm^{-3} atm^{-1}	the current value
NAME	Char	The name of the impurity		the last name specified
NITRIDE	Log	Specifies that the material dependent parameters apply to antimony in silicon nitride		false
OXIDE	Log	Specifies that the material dependent parameters apply to antimony in silicon dioxide		false.
POLYSILI	Log	Specifies that the material dependent parameters apply to antimony in polysilicon		false
Q.SITES	Num	Effective density of segregation sites at a grain boundary	sites/cm^2	the current value
SILICON	Log	Specifies that the material dependent parameters apply to antimony in silicon		false

The ANTIMONY statement is an alias for the IMPURITY statement with an index of four and is used to define or modify the parameters and coefficients associated with antimony as an impurity. Not all of the parameters of the IMPURITY statement apply to antimony and so are not listed here.

IX. Arsenic Statement

The ARSENIC statement is used to input or modify the physical or model coefficients associated with arsenic as a dopant impurity.

ARSENIC
[NAME=<c>] [DONOR] [AT.WT=<n>] [AT.NUMB=<n>] [IONFILE1=<c>] [IONFILE2=<c>]
[((SILICON [FII.0=<n>] [FII.E=<n>] [K.MF=<n>] [K.A=<n>] [K.P=<n>] [(IMPLANT | CHEMICAL) [CTN.0=<n>] [CTN.E=<n>] [CTN.F=<n>]]) | (POLYSILI [ENTROPY=<n>] [HEAT.SEG=<n>] [Q.SITES=<n>] [FII.0=<n>] [FII.E=<n>] [(IMPLANT | CHEMICAL) [CTN.0=<n>] [CTN.E=<n>] [CTN.F=<n>]]) | (OXIDE | NITRIDE | ALUMINUM)
[ELECT.ST=<n>] [DIX.0=<n>] [DIX.E=<n>] [DIM.0=<n>] [DIM.E=<n>] [DIMM.0=<n>] [DIMM.E=<n>]]

Name	Type	Description	Unit	Default
ALUMINUM	Log	Specifies that the material dependent parameters apply to arsenic in aluminum.		false

AT.NUMB	Num	The atomic number of the impurity		the current value
AT.WT	Num	The atomic weight of the impurity	amu	the current value
CHEMICAL	Log	Specifies that the clustering coefficients apply to the impurity from a chemical source.		false
CTN.0	Num	The pre-exponential constant used in calculating the impurity clustering coefficient.	atoms/cm^3	the current value
CTN.E	Num	The activation energy used in calculating the impurity clustering coefficient.	eV	the current value
CTN.F	Num	The power dependence of the concentration used in calculating the impurity clustering coefficient.		the current value
DIM.0	Num	The pre-exponential constant of the diffusion coefficient of the impurity diffusing with singly negative vacancies.	μm^2/min.	the current value
DIM.E	Num	The activation energy of the diffusion coefficient of the impurity diffusing with singly negative vacancies.	eV	the current value
DIMM.0	Num	The pre-exponential constant of the diffusion coefficient of the impurity diffusing with doubly negative vacancies.	μm^2/min.	the current value
DIMM.E	Num	The activation energy of the diffusion coefficient of the impurity diffusing with doubly negative vacancies.	eV	the current value
DIX.0	Num	The pre-exponential constant of the diffusion coefficient of he impurity diffusing with neutral vacancies.	μm^2/min.	the current value
DIX.E	Num	The activation energy of the diffusion coefficient of the impurity diffusing with neutral vacancies.	eV	the current value
DONOR	Log	Specifies that the impurity is a donor in silicon.		the current value
ELECT.ST	Num	The electric stopping power of the impurity in the specified material.	KeV/ μm	the current value
ENTROPY	Num	The entropy factor. Used to calculate the equilibrium segregation factor at polysilicon grain boundaries.		the current value
FII.0	Num	The pre-exponential constant of the fractional partial-interstitialcy contribution.	μm /min$^{-1/2}$	the current value
FII.E	Num	The activation energy of the fractional partial-interstitialcy contribution.	eV	the current value
HEAT.SEG	Num	The activation energy of the equilibrium segregation factor at polysilicon grain boundaries.	eV	the current value
IMPLANT	Log	Specifies that the impurity clustering coefficients apply to the impurity from an implanted source.		false
IONFILE1	Char	Specifies the primary ion implant range data file for implants using the analytic distrbutions. This file will be searched for the range statistics when implanting atomic arsenic.		the last file specified
IONFILE2	Char	Specifies the secondary ion implant range data file for implants using the analytic distributions.		the last file specified

		This file will be searched for the range statistics when implanting the compound ions containing arsenic.		
K.A	Num	Used in R. Reif's epitaxial doping model (see reference in EPITAXY statement). K.a is a thermodynamic constant relating the dopant species concentration in solid silicon and adsorbed layer.	cm	the current value
K.MF	Num	Used in R. Reif's epitaxial doping model (see reference in EPITAXY statement). K.mf is a kinetic coefficient controlling the rate-limiting step of the dopant incorporation process.	cm^{-2} $min.^{1}$ atm^{-1}	the current value
K.P	Num	Used in R. Reif's epitaxial doping model (see reference in EPITAXY statement). K.p is a thermodynamic constant relating the dopant species concentration in solid silicon and gas phase.	cm^{-3} atm^{-1}	the current value
NAME	Char	The name of the impurity.		the last name specified
NITRIDE	Log	Specifies that the material dependent parameters apply to arsenic in silicon nitride.		false
OXIDE	Log	Specifies that the material dependent parameters apply to arsenic in silicon dioxide.		false.
POLYSILI	Log	Specifies that the material dependent parameters apply to arsenic in polysilicon.		false
Q.SITES	Num	Effective density of segregation sites at a grain boundary.	$sites/cm^2$	the current value
SILICON	Log	Specifies that the material dependent parameters apply to silicon.		false.

The ARSENIC statement is an alias for the IMPURITY statement with an index of three and is used to define or modify the parameters and coefficients associated with arsenic as an impurity. Not all of the parameters of the IMPURITY statement apply to arsenic and so are not listed here.

X. Bias Statement

The BIAS statement is used to specify the bias of conductor and semiconductor layers during a Poisson solution initiated by the ELECTRICAL statement.

BIAS
LAYER=<n> ([V.ELECTR=<n>] [DV.ELECTR=<n>]) | (([DIFFUSIO=<n>] [V.MAJORI=<n>] [DV.MAJOR=<n>] [V.MINORI=<n>] [DV.MINOR=<n>]) | [FLOAT])

Name	Type	Description	Unit	Default
DIFFUSIO	Num	The index of the diffused region for which the quasi-Fermi potentials are specified. The parameter is valid only for a semiconductor layer.		All diffused regions in the layer
LAYER	Num	The index of the conductor or semiconductor layer for which a bias is being specified.		
DV.ELECT	Num	The increment for the bias applied to a conductor layer. This parameter is valid only for a conductor	V	0.0

		layer.		
DV.MAJOR	Num	The increment for the quasi-Fermi potential of majority carriers for a diffused region of a semiconductor layer. This parameter is valid only for a semiconductor layer.	V	0.0
DV.MINOR	Num	The increment for the quasi-Fermi potential of minority carriers for a diffused region of a semiconductor layer. This parameter is valid only for a semiconductor layer.	V	0.0
FLOAT	Log	Specifies that a polysilicon layer is to be treated as a neutral dielectric. This parameter is valid only for a polysilicon layer.		false
V.ELECTR	Num	The initial value for the bias applied to a conductor layer. This parameter is valid only for a conductor layer.	V	0.0
V.MAJORI	Num	The initial value for the quasi-Fermi potential of majority carriers for a diffused region of a semiconductor layer. This parameter is valid only for a semiconductor layer.	V	0.0
V.MINORI	Num	The initial value for the quasi-Fermi potential of minority carriers for a diffused region of a semiconductor layer. This parameter is valid only for a semiconductor layer	V	0.0

The BIAS statement specifies the bias of a material layer. One BIAS statement may appear for each conductor layer and for each diffused region of a semiconductor layer. Diffused regions are bounded by material interfaces and metallurgical junctions.

For a semiconductor layer, elimination of the DIFFUSIO parameter applies the specified biases to all diffused regions in the layer. Additional BIAS statements may be included to override these values, which are used as the default values in regions for which specific BIAS statements do not appear.

The increment parameters on the BIAS statement are used to advance the bias values for each Poisson solution, where the number of solutions is controlled by the STEPS parameter on the ELECTRICAL statement.

XI. Boron Statement

The BORON statement is used to input or modify the physical or model coefficients associated with boron as a dopant impurity.

BORON
[NAME=<c>] [ACCEPTOR] [AT.WT=<n>] [AT.NUMB=<n>] [IONFILE1=<c>] [IONFILE2=<c>]
[((SILICON [FII.0=<n>] [FII.E=<n>] [K.MF=<n>] [K.A=<n>] [K.P=<n>]) | (POLYSILI [ENTROPY=<n>] [HEAT.SEG=<n>] [Q.SITES=<n>] [FII.0=<n>] [FII.E=<n>]) | (OXIDE | NITRIDE | ALUMINUM) [ELECT.ST=<n>] [DIX.0=<n>] [DIX.E=<n>] [DIP.0=<n>] [DIP.E=<n>]]

Name	Type	Description	Unit	Default
ACCEPTOR	Log	Specifies that the impurity is an acceptor in silicon.		false
ALUMINUM	Log	Specifies that the material dependent parameters apply to boron in aluminum.		false

AT.NUMB	Num	The atomic number of the impurity.		the current value
AT.WT	Num	The atomic weight of the impurity.	amu	the current value
DIP.0	Num	The pre-exponential constant of the diffusion coefficient of the impurity diffusing with positive vacancies.	μm^2/min.	the current value
DIP.E	Num	The activation energy of the diffusion coefficient of the impurity diffusing with positive vacancies.	eV	the current value
DIX.0	Num	The pre-exponential constant of the diffusion coefficient of the impurity diffusing with neutral vacancies.	μm^2/minute	the current value
DIX.E	Num	The activation energy of the diffusion coefficient of the impurity diffusing with neutral vacancies.	eV	the current value
ELECT.ST	Num	The electric stopping power of the impurity in the specified material.	KeV/ μm	the current value
ENTROPY	Num	The entropy factor. Used to calculate the equilibrium segregation factor at polysilicon grain boundaries.		the current value
FII.0	Num	The pre-exponential constant of the fractional partial-interstitialcy contribution.	$(\mu m/min)^{-1/2}$	the current value
FII.E	Num	The activation energy of the fractional partial-interstitialcy contribution.	eV	the current value.
HEAT.SEG	Num	The activation energy of the equilibrium segregation factor at polysilicon grain boundaries.	eV	the current value
IONFILE1	Char	Specifies the primary ion implant range data file for implants using the analytic distributions. This file will be searched for the range statistics when implanting atomic boron.		the last file specified
IONFILE2	Char	Specifies the secondary ion implant range data file for implants using the analytic distributions. This file will be searched for the range statistics when implanting BF2 ions.		the last file specified
K.A	Num	Used in R. Reif's epitaxial doping model (see reference in EPITAXY statement). K.a is a thermodynamic constant relating the dopant species concentration in solid silicon and adsorbed layer.	cm	the current value
K.MF	Num	Used in R. Reif's epitaxial doping model (see reference in EPITAXY statement). K.mf is a kinetic coefficient controling the rate-limiting step of the dopant incorporation process.	cm^{-2} min^{-1} atm^{-1}	the current value
K.P	Num	Used in R. Reif's epitaxial doping model (see reference in EPITAXY statement). K.p is a thermodynamic constant relating the dopant species concentration in solid silicon and gas phase.	cm^{-3} atm^{-1}	the current value
NAME	Char	The name of the impurity.		the last name specified
NITRIDE	Log	Specifies that the material dependent parameters apply to boron in silicon nitride.		false
OXIDE	Log	Specifies that the material dependent parameters apply to boron in silicon dioxide.		false.

POLYSILI	Log	Specifies that the material dependent parameters apply to boron in polysilicon.		false
Q.SITES	Num	Effective density of segregation sites at a grain boundary.	sites/cm^2	the current value
SILICON	Log	Specifies that the material dependent parameters apply to boron in silicon.		false

The BORON statement is an alias for the IMPURITY statement with an index of one and is used to define or modify the parameters and coefficients associated with boron as an impurity. Not all of the parameters of the IMPURITY statement apply to boron and so are not listedhere.

XII. Comment Statement

The COMMENT statement is used to input a character string to label the following input sequence.

COMMENT [<c>]
or
$ [<c>]

The character string associated with the COMMENT statement is output to the standard output device. If the previous statement was neither another COMMENT statement nor a TITLE statement, then a line feed is issued before the character string is output.

XIII. Deposition Statement

The DEPOSITION statement is used to deposit a specified material on top of the current structure. The material may be doped or undoped.

DEPOSITION
THICKNES=<n>
(SILICON (<111> | <110> | <100>) | POLYSILI TEMPERAT=<n> [PRESSURE=<n> | GRAINSIZ=<n>] | OXIDE | NITRIDE | ALUMINUM)
[DX=<n>] [XDX=<n>] [SPACES=<n>] [MIN.DX=<n>] [CONCENTRATION=<n> (ANTIMONY | ARSENIC | BORON | PHOSPHOR)]

Name	Type	Description	Unit	Default	Synonym
ALUMINUM	Log	Specifies that the material to be deposited is aluminum.		false	
ANTIMONY	Log	Specifies that the deposited material is to be uniformly doped with antimony.		false	SB
ARSENIC	Log	Specifies that the deposited material is to be uniformly doped with arsenic.		false	AS
BORON	Log	Specifies that the deposited material is to be uniformly doped with boron.		false	
CONCENTR	Num	The concentration at which the deposited material is to be uniformly doped.	atoms/cm^3	0.0	
DX	Num	The nominal grid spacing to be used in the deposited layer at the location associated with the XDX parameter.	microns	the nominal dx of the top layer if its material is the	

				same as is being deposited, otherwise, the default dx of the deposited material.
GRAINSIZ	Num	The as-deposited grain size of the deposited polysilicon layer.	microns	calculated from the deposition temperature and pressure
MIN.DX	Num	The minimum grid spacing that can be used in the layer on which the layer is to be deposited.	microns	the last value specified
NITRIDE	Log	Specifies that the material to be deposited is silicon nitride.		false
OXIDE	Log	Specifies that the material to be deposited is silicon dioxide.		false
PHOSPHOR	Log	Specifies that the deposited material is to be uniformly doped with phosphorus.		false
POLYSILI	Log	Specifies that the material to be deposited is poly-crystalline silicon.		false
PRESSURE	Num	The pressure during the deposition of a polysilicon layer.	atm	1.0
SILICON	Log	Specifies that the material to be deposited is single crystal silicon.		false
SPACES	Num	The number of spaces to be used in the deposited layer.		thickness/dx
TEMPERAT	Num	The temperature during deposition of a polysilicon layer.		degrees Centigrade
THICKNES	Num	The thickness of the deposited layer.(unit: microns.)		
XDX	Num	The distance from the surface of the layer at which the nominal grid spacing, DX, applies.	microns	0
<100>	Log	Specifies that the crystalline orientation of the deposited silicon is <100>.		false
<110>	Log	Specifies that the crystalline orientation of the deposited silicon is <110>.		false
<111>	Log	Specifies that the crystalline orientation of the deposited silicon is <111>.		false

The DEPOSITION statement is used to deposit a given thickness of the specified material on top of the existing structure. The material deposited may be either undoped or doped uniformly with one of the availableimpurity types. If the material to be deposited is of the same type as is already present in the top layer of the structure, then the material is added to the existing top layer. If the top layer material is of a different type than that being deposited, then a new layer is created for the deposited material.

If single crystal silicon is being deposited, then the crystalline orientation must also be specified. If polysilicon is being deposited, then the deposition temperature must also be specified. The resulting polysilicon grain size will be calculated from the deposition temperature and pressure unless overridden by the user via the GRAINSIZE parameters.

XIV. Diffusion Statement

The DIFFUSION statement is used to model high temperature diffusion in both oxidizing and non-oxidizing ambients.

DIFFUSION
TIME=<n> TEMPERAT=<n> [T.RATE=<n>] [(GAS.CONC=<n> | SOLIDSOL) (ANTIMONY | ARSENIC | BORON | PHOSPHOR)]
[(DRYO2 | WETO2 | NITROGEN) [PRESSURE=<n>] [P.RATE=<n>] [HCL%=<n>]]
[DTMIN=<n>] [DTMAX=<n>] [ABS.ERR=<n>] [REL.ERR=<n>]

Name	Type	Description	Unit	Default	Synonym
ABS.ERR	Num	Specifies the maximum desired absolute truncation error. Used to control the time step as described below.	cm^{-3}	1.0^{14}	
ANTIMONY	Log	Specifies that the impurity in the ambient gas is antimony.		false	SB
ARSENIC	Log	Specifies that the impurity in the ambient gas is arsenic.		false	AS
BORON	Log	Specifies that the impurity in the ambient gas is boron.		false	
DTMAX	Num	The largest time increment to be used during the solution.	min.	5.0	
DTMIN	Num	The smallest time increment to be used during the solution.	min.	0.005	
DRYO2	Log	Specifies that the ambient gas consists of dry oxygen.		false	
GAS.CONC	Num	The concentration of the specified impurity in the ambient gas at the surface of the structure.	$atoms/cm^3$	0.0	CONCENTRATION
HCL%	Num	The percentage of chlorine present in the ambient gas.	percent	percentage specified in corresponding ambient statement (DryO2, WetO2, Nitrogen))	
NITROGEN	Log	Specifies that the ambient consists of nitrogen (non-oxidizing ambient).		true.)	
P.RATE	Num	The rate of change in the ambient gas pressure.	atm/min.	0.0	
PHOSPHOR	Log	Specifies that the impurity in the ambient gas is phosphorus.	false		
PRESSURE	Num	The pressure of the ambient gas. (See note below.)	atm.	pressure specified in corresponding ambient statement (DryO2, WetO2, Nitrogen))	
REL.ERR	Num	Specifies the maximum desired relative truncation error. Used to		0.5	

		control the time step as described below.		
SOLIDSOL	Log	Sets the concentration of the specified impurity in the ambient gas at the surface of the structure to the solid solubility of the impurity in silicon.		false
TIME	Num	The total elapsed time of the diffusion step being simulated.	min.	
TEMPERAT	Num	The temperature of the ambient at the beginning of the step.	°C	
T.RATE	Num	The rate of change of the ambient temperature.	°C /min.	0.0
WETO2	Log	Specifies that the ambient gas consists of wet oxygen or pyrogenic steam. (See note below.)		false

The DIFFUSION statement simulates impurity diffusion in the structure under a variety of oxidizing and non-oxidizing conditions. At a minimum, only the time and temperature of a step needs to be specified. In this case a non-oxidizing drive-in is assumed. For oxidizing ambients or gaseous predepositions additional parameters need to be specified. The default pressures and chlorine percentages are set previously by the oxidation ambient model cards (e.g. DRYO2, WETO2, NITROGEN),while the defaults of the other optional parameters are set in the GENII key file S3FKY0.

The numerical solution of the diffusion equations requires that the total step time be divided into a number of smaller time increments, dt's, in order to insure sufficient accuracy. There are two mechanisms that control the choice of dt's, one is due to a restriction on interface movement such that no interface moves more than one cell spacing during a dt. The other time step control algorithm has been chosen to give the desired accuracy without using excessive amounts of computation time. Unless the interface control chooses a smaller dt, it will attempt to use a dt equal to that specified by the DTMIN parameter. Sub-sequent dt's are chosen in the following manner.

1. At each point in the current structure a projected concentration is calculated from the previous two solutions.

Cp = C' + (C' - C")*dt/dt'

Where C' is the previous concentration, C" is the concentration before that, and dt' is the previous dt.

2. From the current solution value, C, and the absolute and relative truncation error parameters, an `error' term at each point is then calculated.

Cerr = abs(C - Cp) / (ABS.ERR + abs(C)*REL.ERR)

3. The next dt is then calculated from the following expression.

dtnext = dt * sqrt((1. + dt/dt')/Cerrmax)

Where Cerrmax is the maximum value of Cerr calculated at each point in the structure.

4. A value of dtnext is calculated for each impurity present with the smallest value being the one that is ultimately used.

NOTE: The effective oxidant partial pressure for pyrogenic steam reactors has been found to vary significantly from facility to facility. It is recommended that the user set the default pressure for WetO2 to a value that gives the best agreement with measured oxide thicknesses from his facility.

XV. DryO2 Statement

The DRYO2 statement allows the user to modify the coefficients used to model the oxidation of the various materials under dry ambient oxidation conditions.

DRYO2
[(<111> | <110> | <100>) [LIN.L.0=<n>] [LIN.L.E=<n>] [LIN.H.0=<n>] [LIN.H.E=<n>] [THINOX.0=<n>] [THINOX.E=<n>] [THINOX.L=<n>]] [PAR.L.0=<n>] [PAR.L.E=<n>] [PAR.H.0=<n>] [PAR.H.E=<n>] [LIN.BREA=<n>] [PAR.BREA=<n>] [LIN.PDEP=<n>] [PAR.PDEP=<n>] [PRESSURE=<n>] [HCL%=<n>] [GAMMA.0=<n>] [GAMMA.E=<n>] [DELTA.0=<n>] [DELTA.E=<n>] [EXP.0=<n>] [EXP.E=<n>] [NIOX.0=<n>] [NIOX.E=<n>] [NIOX.F=<n>] [CL.ROW=<n> [CL.PCT=<n>] CL.COLUM=<n> [CL.TEMPE=<n>] [CL.DEP.L=<n>] [CL.DEP.P=<n>]]

Name	Type	Description	Unit	Default
CL.COLUM	Num	The column number in the table of coefficients used to calculate the chlorine dependence of the oxidation rates.		the current value
CL.DEP.L	Num	The coefficient modifying the linear oxidation rate in the presence of chlorine at the specified row and column.		the current value
CL.DEP.P	Num	The coefficient modifying the parabolic oxidation rate in the presence of chlorine at the specified row and column.		the current value
CL.PCT	Num	The percentage of chlorine for which the coefficients in the specified row are valid.	percent	the current value
CL.ROW	Num	The row number in the table of coefficients used to calculate the chlorine dependence of the oxidation rates.		the current value
CL.TEMPE	Num	The temperature for which the coefficients in the specified column are valid.	°C	the current value
DELTA.0	Num	The pre-exponential factor of the delta coefficient used in calculating the impurity concentration dependence of the parabolic oxidation rate.	cm^3/atom.	the current value
DELTA.E	Num	The activation energy of the delta coefficient used in calculating the impurity concentration dependence of the parabolic oxidation rate.	eV	the current value
EXP.0	Num	The pre-exponential factor of the exponent used in calculating the impurity concentration dependence of the parabolic oxidation rate.		the current value
EXP.E	Num	The activation energy of the exponent used in calculating the impurity concentration dependence of the parabolic oxidation rate.	eV	the current value
GAMMA.0	Num	The pre-exponential factor of the gamma coefficient used in calculating the impurity concentration dependence of the linear oxidation rate.		the current value
GAMMA.E	Num	The activation energy of the gamma coefficient used in calculating the impurity concentration dependence of the linear oxidation rate.	eV	the current value
HCL%	Num	The default percentage of chlorine present in the ambient.	percent	the current value
LIN.BREA	Num	The temperature at which the temperature dependence of the linear oxidation rate changes.	°C	the current value

LIN.H.0	Num	The pre-exponential constant of the linear oxidation rate for temperatures above the breakpoint set by L.BREAKP.	microns/min.	the current value
LIN.H.E	Num	The activation energy of the linear oxidation rate for temperatures above the breakpoint set by L.BREAKP.	eV	the current value
LIN.L.0	Num	The pre-exponential constant of the linear oxidation rate for temperatures below the breakpoint set by L.BREAKP.	microns/min.	the current value
LIN.L.E	Num	The activation energy of the linear oxidation rate for temperatures below the breakpoint set by L.BREAKP.	eV	the current value
LIN.PDEP	Num	The pressure dependence factor for the linear oxidation rate.		the current value
NIOX.0	Num	The pre-exponential constant used to determine the oxidation rate of silicon nitride.	microns.	the current value
NIOX.E	Num	The activation energy used to determine the oxidation rate of silicon nitride.	eV	the current value
NIOX.F	Num	The exponent factor used to determine the oxidation rate of silicon nitride.		the current value
PAR.BREA	Num	The temperature at which the temperature dependence of the parabolic oxidation rate changes.	°C	the current value
PAR.H.0	Num	The pre-exponential constant of the parabolic oxidation rate for temperatures above the breakpoint set by P.BREAKP.	microns^2/min.	the current value
PAR.H.E	Num	The activation energy of the parabolic oxidation rate for temperatures above the breakpoint set by P.BREAKP.	eV	the current value
PAR.L.0	Num	The pre-exponential constant of the parabolic oxidation rate for temperatures below the breakpoint set by P.BREAKP.	microns^2/min.	the current value
PAR.L.E	Num	The activation energy of the parabolic oxidation rate for temperatures below the breakpoint set by P.BREAKP.	eV	the current value.
PAR.PDEP	Num	The pressure dependence factor for the parabolic oxidation rate.		the current value
PRESSURE	Num	The default ambient pressure.	atm.	the current value
THINOX.0	Num	The pre-exponential constant of the thin oxide growth rate parameter.	microns/min.	the current value
THINOX.E	Num	The activation energy of the thin oxide growth rate parameter.	eV	the current value
THINOX.L	Num	The characteristic length of the thin oxide growth rate parameter.	microns	the current value
<100>	Log	Specifies that the linear growth rate and thin oxide growth rate parameters apply to <100> orientation silicon.		false
<110>	Log	Specifies that the linear growth rate and thin oxide growth rate parameters apply to <110> orientation silicon.		false.
<111>	Log	Specifies that the linear growth rate and thin oxide growth rate parameters apply to <111> orientation		false

silicon.

The three oxidation model statements, DRYO2, WETO2, and NITROGEN, use identical parameters, differing only in the values assigned. The parameters NIOX.C, NIOX.E, and NIOX.F are used in modeling the oxidation of silicon nitride while the others deal with the oxidation of single and polycrystalline silicon.

The effects of chlorine in the ambient gas on the oxidation rate of silicon are currently modeled by an empirical expression whose only variable is defined by the L.CLDEP and P.CLDEP for the linear and parabolic rates respectively. To date no convenient function is available to calculate the chlorine dependence as a function of temperature and amount of chlorine present, therefor a table of values defines the chlorine dependence factors at those temperatures and percentages for which reliable data is available. For those temperatures and chlorine percentages between the values in the table, linear interpolation is employed to calculate the value used. For temperatures or percentages outside the range of values present in the table, the values whose conditions most nearly match the current conditions are used. For example, if the current conditions are a temperature of 1175 degrees with three percent chlorine, but the highest temperature entry in the table is 1150 degrees and the nearest chlorine percentages are for two and four percent, then a value halfway between the values at 1150 degrees and two and four percent chlorine will be used.

XVI. Electrical Statement

The ELECTRICAL statement begins a series of numerical solutions of Poisson's equation for the current structure.

ELECTRICAL
[STEPS=<n>] [EXTENT=<n>] [TEMPERAT=<n>] [ERROR=<n>] [MAX.ITER=<n>] [FILE.OUT=<c>]

Name	Type	Description	Unit	Default
ERROR	Num	The allowed relative error between successive approximations during the iterative solution of Poisson's equation.		1×10^{-4}
EXTENT	Num	The distance by which the bottom layer of the structure is extended for the numerical solution of Poisson's equation. This extension is necessary to allow for the proper treatment of depletion regions which extend beyond the bottom of the simulated structure.	microns	0.0
FILE.OUT	char	The name of the file to which the results of the electrical calculations are to be output. The total hole and electron concentrations and their respective conductivities and resistivities are normally written to the standard output, but if a file is specified, they are also written to that file. The potential, net active impurity concentration and the distance from the surface at each node are also written to the file.		
MAX.ITER	Num	The maximum number of iterations allowed for each solution of Poisson's equation.		50
STEPS	Num	The number of bias steps for which Poisson's equation is solved.		1
TEMPERAT	Num	The device temperature used during the solutions of Poisson's equation.	°C	26.84

The ELECTRICAL statement performs the number of solutions of Poisson's equation specified by the STEPS parameter for the current physical structure. The solution region can be extended below the structure used for process simulation by using the EXTEND parameter. For a structure having an insulator layer at the top or bottom, reflection symmetry is used as the boundary condition at the associated external boundary.

Insulator layers in the structure are treated as charge-neutral dielectrics. Conductor layers are treated as regions having constant specified bias. Semiconductor layers have constant specified quasi-Fermi potentials for electrons and holes within each diffused region. Polysilicon layers can also be treated as charge-neutral dielectric layers. The above bias information is specified through a series of BIAS statements which follow the ELECTRICAL statement and are terminated by an END.ELECTRICAL statement.

For each Poisson solution, the total electron and hole concentrations, conductivities, and sheet resistances are calculated and printed for all diffused regions in the semiconductor layers.

XVII. End.Electrical Statement

The END.ELEC statement terminates a sequence of BIAS statements associated with the ELECTRIC statement.

END.ELEC [<c>]

XVIII. Epitaxy Statement

The EPITAXY statement simulates the epitaxial growth of silicon layers.

EPITAXY
TEMPERAT=<n> TIME=<n> (GROWTH.R=<n> | PP.SILAN=<n>) [(ANTIMONY | ARSENIC | BORON | PHOSPHOR) (CONCENTR=<n> | PP.DOPAN=<n>) [DTMIN=<n>] [DTMAX=<n>] [ABS.ERR=<n>] [REL.ERR=<n>]

Name	Type	Description	Unit	Default	Synonym
ABS.ERR	Num	Specifies the maximum desired absolute truncation error. Used to control the time step as described below.	cm^{-3}	1.0^{14}	
ANTIMONY	Log	Specifies that the impurity in the ambient gas is antimony.		false	SB
ARSENIC	Log	Specifies that the impurity in the ambient gas is arsenic.		false	AS
BORON	Log	Specifies that the impurity in the ambient gas is boron.		false	
CONCENTR	Num	The concentration of the specified impurity in the ambient gas at the surface of the structure.	atoms/ cm^3	0.0	GAS.CON C
DTMAX	Num	The largest time increment to be used during the solution.	min.	5.0	
DTMIN	Num	The smallest time increment to be used during the solution.	min.	0.005	
GROWTH.R	Num	The growth rate of the epitaxial layer.	micron s/min.		
PHOSPHOR	Log	Specifies that the impurity in the ambient gas is phosphorus.		false	
PP.DOPAN	Num	Specifies the input dopant partial pressure. This is	atm	0.0	

		approximately equal to the dopant input flow rate divided by the hydrogen carrier input flow rate. See the R. Reif reference below.		
PP.SILAN	Num	Specifies the input silane partial pressure. This is approximately equal to the silane input flow rate divided by the hydrogen carrier input flow rate. See the R. Reif reference below.	atm	0.0
REL.ERR	Num	Specifies the maximum desired relative truncation error. Used to control the time step as described below.		0.5
TEMPERAT	Num	The temperature at the beginning of the step.	°C	
TIME	Num	The total elapsed time of the epitaxy step being simulated.	min.	

The EPITAXY statement is used to grow a layer of single crystal silicon on top of the current structure. The epitaxial layer may be either doped or undoped. To grow an epitaxial layer, the top layer must be single crystal silicon.

The growth rate used in the simulation may be specified in one of two ways. The first is to explicitly specify it with the GROWTH.R parameter. The second is to specify the input partial pressure of silane with the PP.SILAN parameter causing the rate to be determined from the product of the partial pressure and the mass transport coefficient of silane in hydrogen as specified by the SILICON statement. (Reference, `Computer Simulation in Silicon Epitaxy', by R. Reif and R. W. Dutton, J. Electrochem. Soc., Vol. 128, No. 4, April 1981, pp 909-918.)

AnaLogous to the growth rate, the impurity concentration in doped epi-layers may be specified in one of two ways. The first is to explicitly specify the surface concentration with the CONCENTR parameter. The second is to specify the input partial pressure of the dopant with the PP.DOPAN parameter. The surface concentration is then calculated as a function of the partial pressure, time increment, growth rate, and the mass transport and kinetic coefficients, K.a, K.p, and K.mf as specified by the SILICON statement. (See the previous reference.)

The numerical solution of the diffusion equations requires that the total step time be divided into a number of smaller time increments, dt's, in order to insure sufficient accuracy. There are two mechanisms that control the choice of dt's, one is due to a restriction on interface movement such that no interface moves more than one cell spacing during a dt. The other time step control algorithm has been chosen to give the desired accuracy without using excessive amounts of computation time. Unless the interface control chooses a smaller dt, it will attempt to use a dt equal to that specified by the DTMIN parameter. Sub-sequent dt's are chosen in the following manner.

1. At each point in the current structure a projected concentration is calculated from the previous two solutions.

Cp = C' + (C' - C")*dt/dt'

Where C' is the previous concentration, C" is the concentration before that, and dt' is the previous dt.

2. From the current solution value, C, and the absolute and relative truncation error parameters, an `error' term at each point is then calculated.

Cerr = abs(C - Cp) / (ABS.ERR + abs(C)*REL.ERR)

3. The next dt is then calculated from the following expression.

dtnext = dt * sqrt((1. + dt/dt')/Cerrmax)

Where Cerrmax is the maximum value of Cerr calculated at each point in the structure.

4. A value of dtnext is calculated for each impurity present with the smallest value being the one that is ultimately used.

XIX. Etch Statement

The ETCH statement is used to etch a specified material from the top of the current structure.

ETCH
(SILICON | POLYSILI | OXIDE | NITRIDE | ALUMINUM) [(THICKNES=<n> | ALL)]

Name	Type	Description	Unit	Default	Synonym
ALL	Log	Specifies that all of the specified material is to be etched.		true	
ALUMINUM	Log	Specifies that the material to be etched is aluminum.		false	
NITRIDE	Log	Specifies that the material to be etched is silicon nitride.		false	
OXIDE	Log	Specifies that the material to be etched is silicon dioxide.		false	
POLYSILI	Log	Specifies that the material to be etched is poly-crystalline silicon.		false	
SILICON	Log	Specifies that the material to be etched is single crystal silicon.		false	
THICKNESS	Num	The amount of the material to be etched.	microns	the surface layer thickness	AMOUNT

The ETCH statement is used to etch a specified amount of the specified material from the top of the existing structure. If the material at the top of the structure is not the material specified then no etching takes place. If the amount to be etched is not specified then the entire layer is removed.

XX. Grid Statement

The GRID statement specifies the grid spacing parameters for one or more of the layers in a structure. For the first layer, the thickness may also be extended.

GRID
LAYER.<n> [THICKNES=<n>] [DX=<n>] [MIN.DX=<n>] [XDX=<n>] [SPACES=<n>]

Name	Type	Description	Unit	Default
DX	Num	The nominal grid spacing in to be used in the specified layer(s) at the location associated with the XDX parameter.	microns	The current nominal grid spacing
LAYER.<n>	Log	Specifies that the grid parameters are to apply to the n'th layer of the structure.		false
MIN.DX	Num	The minimum grid spacing that can be used in the specified layer(s).	microns	The current minimum grid spacing
SPACES	Num	The number of spaces to be used in the specified layer(s).		The current number of spaces in the layer
THICKNESS	Num	The thickness of the first layer. If the specified thickness is greater than the current layer thickness, then additional material is added to the	microns	The current layer thickness

		bottom of the layer. The value specified must be greater than or equal to the current thickness.		
XDX	Num	The distance from the surface of the layer at which the nominal grid spacing, DX, applies.	microns	The last value specified

The GRID statement is used primarily to change the grid spacing of one or more layers of the current structure. In the case of the first, or bottom layer, the GRID statement may be used to extend the depth of the layer by adding additional material to the bottom of the structure. In this case, the impurity concentration at the bottommost cell in the structure is used uniformly in the added region.

XXI. Implant Statement

The IMPLANT statement is used to simulate the ion-implantation of impurities into the structure. Four types of implantation models are available, a numerical method based on the Boltzman transport equation, and three analytical methods based on simple Gaussian, two sided Gaussian, or Pearson type-IV distributions.

IMPLANT
DOSE=<n> ENERGY=<n> (ANTIMONY | ARSENIC | BF2 | BORON | PHOSPHOR) (GAUSSIAN | 2-GAUSSI | PEARSON | (BOLTZMAN [MINSTEPS=<n>] [AT.WT=<n>] [AT.NUMB=<n>]))

Name	Type	Description	Unit	Default	Synonym
ANTIMONY	Log	Specifies that the ion to be implanted is antimony.		false	SB
ARSENIC	Log	Specifies that the ion to be implanted is arsenic.		false	AS
AT.NUMB	Num	The atomic number of the ion to be implanted.		The last value specified in the corresponding impurity coefficient statement	
AT.WT	Num	The atomic weight of the ion to be implanted.	amu	The last value specified in the corresponding impurity coefficient statement	AT.MASS
BF2	Log	Specifies that the ion to be implanted is boron-difluoride.		false	
BOLTZMAN	Log	Specifies that the Boltzman transport model is to be used in simulating the implantation.		false	
BORON	Log	Specifies that the ion to be implanted is atomic boron.		false	
DOSE	Num	The implanted dose.	atoms/cm^2		
ENERGY	Num	The energy of the implant beam.	thousand eV		
GAUSSIAN	Log	Specifies that a simple Gaussian distribution is to be used to model the implanted profile.		false	
MINSTEPS	Num	The minimum number of steps between each grid point used in calculating the energy distribution during the solution		5.0	

		of the Boltzman transport equation.	
PEARSON	Log	Specifies that a Pearson type-IV distribution is to be used to model the implanted profile.	true, if no other model is specified
PHOSPHOR	Log	Specifies that the ion to be implanted is phosphorus.	false
2-GAUSSI	Log	Specifies that a two sided Gaussian distribution is to be used to model the implanted profile.	false

The IMPLANT statement is used to simulate ion-implantation of impurities into the structure. Four different ion-implantation models are available.

When the BOLTZMANN option is selected, the implanted ion distribution is calculated by a numerical solution of the Boltzmann transport equation [1]. In this method, the momentum distribution of the implanted ion is determined at each depth in the target. Then distribution in energy and angle is represented numerically by a two-dimensional array (default size 15 x 8).

The calculation proceeds starting from the surface, where the momentum distribution is known to be a delta function (mono-energetic beam moving normal to the target surface). A knowledge of the scattering cross section for both two-body atomic and electronic interactions, together with the transport equations, is then sufficient to determine how the momentum distribution evolves with depth. Material discontinuities are simple to handle, since only the cross sections change as the ions cross any interface. When any ion scatters to an energy less than about 5% of the initial energy, or when an ion is scattered back toward the target surface, that ion is considered stopped at that depth and becomes part of the range distribution.The calculation proceeds until the concentration of the implanted profile drops to 10^{-5} of its peak value.

The other three models are based on fitting the as-implanted distribution to an analytical function. The three functions available are a simple Gaussian, a two sided Gaussian, or a Pearson type-IV distribution. The necessary moments, or range statistics, are read from the implant moment data file specified via the appropriate impuritys statement.

XXII. Impurity Statement

The IMPURITY statement is used to input or modify the physical or model coefficients associated with a dopant impurity.

IMPURITY

INDEX=<n> [NAME=<c>] [(DONOR | ACCEPTOR)] [AT.WT=<n>] [AT.NUMB=<n>] [IONFILE1=<c>] [IONFILE2=<c>]

[((SILICON [FII.0=<n>] [FII.E=<n>] [K.MF=<n>] [K.A=<n>] [K.P=<n>] [MISFITST=<n>] [CD=<n>] [MSF111FA=<n>] [MSF110FA=<n>] [MSF100FA=<n>] [DAMAGEST=<n>] [NE.0=<n>] [NE.E=<n>] [(IMPLANT | CHEMICAL) [CTN.0=<n>] [CTN.E=<n>] [CTN.F=<n>]]) | (POLYSILI [ENTROPY=<n>] [HEAT.SEG=<n>] [Q.SITES=<n>] [FII.0=<n>] [FII.E=<n>] [(IMPLANT | CHEMICAL) [CTN.0=<n>] [CTN.E=<n>] [CTN.F=<n>]]) | (OXIDE | NITRIDE | ALUMINUM)

[ELECT.ST=<n>] [DIX.0=<n>] [DIX.E=<n>] [DIM.0=<n>] [DIM.E=<n>] [DIMM.0=<n>] [DIMM.E=<n>] [DIP.0=<n>] [DIP.E=<n>]]

Name	Type	Description	Unit	Default
ACCEPTOR	Log	Specifies that the impurity is an acceptor in		false

		silicon.		
ALUMINUM	Log	Specifies that the material dependent parameters apply to the impurity in aluminum.		false
AT.NUMB	Num	The atomic number of the impurity.		the current value
AT.WT	Num	The atomic weight of the impurity.	amu	the current value
CD	Num	This parameter is used to calculate the temperature dependent part of the expression for bandgap narrowing due to lattice misfit strain from high concentrations of phosphorus.	atoms/cm^3 °C^2	current value
CHEMICAL	Log	Specifies that the clustering coefficients apply to the impurity from a chemical source.		false
CTN.0	Num	The pre-exponential constant used in calculating the impurity clustering coefficient.	atoms/cm^3	the current value
CTN.E	Num	The activation energy used in calculating the impurity clustering coefficient.	eV	the current value
CTN.F	Num	The power dependence of the concentration used in calculating the impurity clustering coefficient.		the current value
DAMAGEST	Num	The factor in the implant dose dependent expression for calculating the bandgap narrowing due to the residual damage of phosphorus implants.	eV-cm$^{1/2}$	the current value
DIM.0	Num	The pre-exponential constant of the diffusion coefficient of the impurity diffusing with singly negative vacancies.	microns^2/ min.	the current value
DIM.E	Num	The activation energy of the diffusion coefficient of the impurity diffusing with singly negative vacancies.	eV	the current value
DIMM.0	Num	The pre-exponential constant of the diffusion coefficient of the impurity diffusing with doubly negative vacancies.	microns^2/ min.	the current value
DIMM.E	Num	The activation energy of the diffusion coefficient of the impurity diffusing with doubly negative vacancies.	eV	the current value
DIP.0	Num	The pre-exponential constant of the diffusion coefficient of the impurity diffusing with positive vacancies.	microns^2/ min.	the current value
DIP.E	Num	The activation energy of the diffusion coefficient of the impurity diffusing with positive vacancies.	eV	the current value
DIX.0	Num	The pre-exponential constant of the diffusion coefficient of the impurity diffusing with neutral vacancies.	microns^2/ min.	the current value
DIX.E	Num	The activation energy of the diffusion coefficient of the impurity diffusing with neutral vacancies.	eV	the current value
DONOR	Log	Specifies that the impurity is a donor in silicon.		the current value
ELECT.ST	Num	The electric stopping power of the impurity in the specified material.	KeV/micro n	the current value
ENTROPY	Num	The entropy factor. Used to calculate the equilibrium segregation factor at polysilicon grain boundaries.		the current value
FII.0	Num	The pre-exponential constant of the fractional partial-interstitialcy contribution.	(microns/ minute)$^{-1/2}$	the current value

<table>
<tr><td>FII.E</td><td>Num</td><td>The activation energy of the fractional partial-interstitialcy contribution.</td><td>eV</td><td>the current value</td></tr>
<tr><td>HEAT.SEG</td><td>Num</td><td>The activation energy of the equilibrium segregation factor at polysilicon grain boundaries.</td><td>eV</td><td>the current value</td></tr>
<tr><td>IMPLANT</td><td>Log</td><td>Specifies that the impurity clustering coefficients apply to the impurity from an implanted source.</td><td></td><td>false</td></tr>
<tr><td>IONFILE1</td><td>Char</td><td>Specifies the primary ion implant range data file for implants using the analytic distributions. This file will be searched for the range statistics when implanting the atomic ion of this impurity.</td><td></td><td>the last file specified</td></tr>
<tr><td>IONFILE2</td><td>Char</td><td>Specifies the secondary ion implant range data file for implants using the analytic distributions. This file will be searched for the range statistics when implanting the compound ions containing this impurity.</td><td></td><td>the last file specified</td></tr>
<tr><td>K.A</td><td>Num</td><td>Used in R. Reif's epitaxial doping model (see reference in EPITAXY statement). K.a is a thermodynamic constant relating the dopant species concentration in solid silicon and adsorbed layer.</td><td>cm</td><td>the current value</td></tr>
<tr><td>K.MF</td><td>Num</td><td>Used in R. Reif's epitaxial doping model (see reference in EPITAXY statement). K.mf is a kinetic coefficient controling the rate-limiting step of the dopant incorporation process.</td><td>cm^{-2} min^{-1} atm^{-1}</td><td>the current value</td></tr>
<tr><td>K.P</td><td>Num</td><td>Used in R. Reif's epitaxial doping model (see reference in EPITAXY statement). K.p is a thermodynamic constant relating the dopant species concentration in solid silicon and gas phase.</td><td>cm^{-3} atm^{-1}</td><td>the current value</td></tr>
<tr><td>MISFITST</td><td>Num</td><td>The prefactor in the high concentration dependent expression for calculating the bandgap narrowing due to the lattice misfit strain from high concentrations of phosphorus.</td><td>eV volts-cm^{-3}</td><td>the current value</td></tr>
<tr><td>MSF100FA</td><td>Num</td><td>The orientation factor in <100> orientation silicon for bandgap narrowing due to lattice misfit strain from high concentrations of phosphorus.</td><td></td><td>the current value</td></tr>
<tr><td>MSF110FA</td><td>Num</td><td>The orientation factor in <110> orientation silicon for bandgap narrowing due to lattice misfit strain from high concentrations of phosphorus.</td><td></td><td>the current value</td></tr>
<tr><td>MSF111FA</td><td>Num</td><td>The orientation factor in <111> orientation silicon for bandgap narrowing due to lattice misfit strain from high concentrations of phosphorus.</td><td></td><td>the current value</td></tr>
<tr><td>NAME</td><td>Char</td><td>The name of the impurity.</td><td></td><td>the last name specified</td></tr>
<tr><td>NE.0</td><td>Num</td><td>The pre-exponential constant for Ne, the concentration at which the P+V= pairs disassociate. Used to calculate the diffusivity of phosphorus at high concentrations.</td><td>$atoms/cm^3$</td><td>the current value</td></tr>
<tr><td>NE.E</td><td>Num</td><td>The activation energy for calculating Ne, the concentration at which the P+V= pairs disassociate. Used to calculate the diffusivity of</td><td>eV</td><td>the current value</td></tr>
</table>

		phosphorus at high concentrations.		
NITRIDE	Log	Specifies that the material dependent parameters apply to the impurity in silicon nitride.		false
OXIDE	Log	Specifies that the material dependent parameters apply to the impurity in silicon dioxide.		false
POLYSILI	Log	Specifies that the material dependent parameters apply to the impurity in polysilicon.	false	
Q.SITES	Num	Effective density of segregation sites at a grain boundary.	sites/cm^2	the current value
SILICON	Log	Specifies that the material dependent parameters apply to the impurity in single crystal silicon.		false

The IMPURITY statement is used to input or modify the coefficients and parameters that define a given impurity. Four impurities are defined, boron, phosphorus, arsenic, and antimony. These impurities each have their own impurity coefficient statements which are aliases of the general IMPURITY statement.

XXIII. Initialize Statement

The INITIALIZE statement, as it's name implies, is used to set up the initial coefficients and structure to be used in the processing steps that follow.

INITIALIZE
[(COEFFICI=<c> | FIRSTIME)] [STRUCTUR=<c>] [MIN.DX=<n>] [SAVESTEP] [THICKNES=<n>] [DX=<n>] [XDX=<n>] [SPACES=<n>]
[(SILICON (<111> | <110> | <100>) | POLYSILI (GRAINSIZ=<n> | (TEMPERAT=<n> [PRESSURE=<n>])) | OXIDE | NITRIDE | ALUMINUM) [CONCENTR=<n> (ANTIMONY | ARSENIC | BORON | PHOSPHOR)]]

Name	Type	Description	Unit	Default	Synonym
ALUMINUM	Log	Specifies that aluminum is the material in the first layer.		false	
ANTIMONY	Log	Specified that the initial structure is to be doped uniformly with antimony.		false	SB
ARSENIC	Log	Specifies that the initial structure is to be doped uniformly with arsenic.		false	AS
BORON	Log	Specifies that the initial structure is to be doped uniformly with boron.		false	
COEFFICI	Char	The name of the file containing the physical coefficients to be used by the program.		S3cof0	
CONCENTR	Num	The impurity concentration at which the structure is to be uniformly doped.	atoms/cm^3	0.0	
DX	Num	The nominal grid spacing to be used in the first layer of the structure at the location specified by XDX.	microns	That of the first layer of the input structure file otherwise, the default for the material in the first	

				layer
FIRSTIME	Log	Indicates that no coefficient file exists. Used the first time the program is executed to create the default coefficient file.		false
GRAINSIZ	Num	Specifies the polysilicon grain size.	microns	
MIN.DX	Num	The minimum grid spacing to be used in the first layer of the structure.	microns	That of the first layer of the input structure file otherwise, 0.001
NITRIDE	Log	Specifies that silicon nitride is the material in the first layer.		false
OXIDE	Log	Specifies that silicon dioxide is the material in the first layer.		false
PHOSPHOR	Log	Specifies that the initial structure is to be doped uniformly with phosphorus.		false
POLYSILI	Log	Specifies that polycrystalline silicon is the material in the first layer.		false
PRESSURE	Num	Specifies the polysilicon deposition pressure.	atm	1.0
SAVESTEP	Log	Causes the structure to be saved in the file S3sav0 after each step in which the structure is modified.		false
SILICON	Log	Specifies that single crystal silicon is the material in the first layer.		false
SPACES	Num	The number of spaces to be used in the layer.		thickness/dx if no structure is input otherwise, the current number of spaces
STRUCTUR	Char	The name of the file containing the initial structure information.		
TEMPERAT	Num	Specifies the polysilicon deposition temperature.	°C	
THICKNES	Num	The thickness of the first layer of the initial structure.	microns	That of the first layer of the input structure file otherwise, none
XDX	Num	The distance from the top of the first layer at which the nominal grid spacing applies.	microns	That of the first layer of the input structure file otherwise, 0.0
<100>	Log	Specifies that the crystalline orientation of the material in the first layer is <100>.		false
<110>	Log	Specifies that the crystalline orientation of the material in the first layer is <110>.		false
<111>	Log	Specifies that the crystalline orientation of the material in the first		false

layer is <111>.

An INITIALIZE statement is required in every SUPREM-III input sequence and it must preceed all other statements except for TITLE or COMMENT statements. At the start of execution the SUPREM-III program contains no information about any of the materials or impurities that may be used in the processing sequence. All of the physical and model coefficients and any initial structure information is contained in one or two files and must be read into the programs internal storage before processing can proceed. Normally, all of the coefficient information is contained in a default file, S3COF0. If this is the case, and if a coefficient file is not specified in the INITIALIZE statement, the data is read from the default coefficient file.

The same is true with the structure information, an initial structure of at least one layer of material must be present before execution can continue. A previously defined structure of arbitrary complexity can be input from a file specified by the STRUCTUR parameter. The other parameters of the INITIALIZE statement may be used to redefine the structure input from a file if the structure has only a single layer of material or, if no structure file is input, they may be used to set up the initial layer.

If no coefficient file is present, the FIRSTIME parameter must be specified and all of the needed coefficients explicitly specified by subsequent statements before processing statements can be executed. As it's name implies, the FIRSTIME parameter should only be needed the first time the program is brought up at a new installation.

XXIV. Loadfile Statement

The LOADFILE statement is used to input either a new structure to be processed, the physical and model coefficients to be used by the program, or both.

LOADFILE
FILENAME=<c> (ALL | COEFFICI | STRUCTUR)

Name	Type	Description	Default	Synonym
ALL	Log	Specifies that both the structure information and the model coefficients are to be input from the specified file.	false	
COEFFICI	Log	Specifies that the coefficient information is to be input from the specified file.	false	
FILENAME	Char	The name of the file from which the specified information is to be read.		NAME
STRUCTUR	Log	Specifies that the information describing the structure is to be input from the specified file.	false	

The LOADFILE statement inputs two classes of information about the process that is to be simulated. The first class is the physical structure and impurity distributions of the materials to be simulated. This file is used as the starting point for subsequent processing steps. The other class of information consists of all of the physical and model parameters or coefficients used by the program.

A LOADFILE statement may appear at any point in a processing sequence after the INITIALIZE statement and before the STOP statement. If both structure and coefficient information are to be input, it is recommended that an INITIALIZE statement be used instead of LOADFILE.

XXV. Material Statement

The MATERIAL statement is used to input or modify the characteristics of a layer material. The program is presently configured to handle up to ten different material types. Materials with index numbers one through five are defaulted to silicon, silicon dioxide, polysilicon, silicon nitride, and aluminum,

respectively. The parameter values for the defaulted materials may also be accessed via the SILICON, OXIDE, POLYSILI, NITRIDE, and ALUMINUM statements.

MATERIAL
[INDEX=<n>] [NAME=<c>] [DX.DEFAU=<n>] [(SEMICOND | CONDUCTO | INSULATO)] [SPECIES=<n>] [DENSITY=<n>] [AT.WT.1=<n>] [AT.WT.2=<n>] [AT.WT.3=<n>] [AT.NUM.1=<n>] [AT.NUM.2=<n>] [AT.NUM.3=<n>] [ABUND.1=<n>] [ABUND.2=<n>] [ABUND.3=<n>] [DIFX.0=<n>] [DIFX.E=<n>] [DIMX.0=<n>] [DIFM.E=<n>] [DIMMX.0=<n>] [DIFMM.E=<n>] [DIFP.0=<n>] [DIFP.E=<n>] [NI.0=<n>] [NI.E=<n>] [NI.F=<n>] [DEFECTLN=<n>] [OEDK.0=<n>] [OEDK.E=<n>] [OED.RATE=<n>] [100.OEDF=<n>] [110.OEDF=<n>] [111.OEDF=<n>] [GSZ.H.0=<n>] [GSZ.H.E=<n>] [GSZ.L.0=<n>] [GSZ.L.E=<n>] [MIN.GRAI=<n>] [TEMP.BRE=<n>] [RATIO.0=<n>] [RATIO.E=<n>] [GEO.FACT=<n>] [GBE.0=<n>] [GBE.E=<n>] [TAU.0=<n>] [TAU.E=<n>] [AFFINITY=<n>] [WORK.FUN=<n>] [EPSILONF=<n>] [N.VALENC=<n>] [N.CONDUC=<n>] [BAND.GAP=<n>] [K.M=<n>]

Name	Type	Description	Unit	Default
ABUND.1	Num	The relative abundance of element one in the material. The sum of all abundances for a material must equal one.		the current value
ABUND.2	Num	The relative abundance of element two in the material. The sum of all abundances for a material must equal one.		the current value
ABUND.3	Num	The relative abundance of element three in the material. The sum of all abundances for a material must equal one.		the current value
AFFINITY	Num	The electron affinity of the material.	eV	the current value
AT.NUM.1	Num	The atomic number of element one in the material.		the current value
AT.NUM.2	Num	The atomic number of element two in the material.		the current value
AT.NUM.3	Num	The atomic number of element three in the material.		the current value
AT.WT.1	Num	The atomic weight of element one in the material.	amu	the current value
AT.WT.2	Num	The atomic weight of element two in the material.	amu	the current value
AT.WT.3	Num	The atomic weight of element three in the material.	amu	the current value
BAND.GAP	Num	The band gap of the material.	eV	the current value
CONDUCTO	Num	Specifies that the material is a conductor.		false
DEFECTLN	Num	The decay length of point defects in the material.	microns	the current value
DENSITY	Num	The density of the material.	grams/cm^3	the current value.
DIFM.0	Num	The pre-exponential constant used in the calculation the component of the self-diffusivity due to diffusion with singly negative vacancies.	microns^2/min.	the current value
DIFM.E	Num	The activation energy used in the calculation the component of the self-diffusivity due to diffusion with singly negative vacancies.	eV	the current value
DIFMM.0	Num	The pre-exponential constant used in the calculation of the component of the self-diffusivity due to diffusion with doubly negative	microns^2/min.	the current value

		vacancies.		
DIFMM.E	Num	The activation energy used in the calculation the component of the self-diffusivity due to diffusion with doubly negative vacancies.	eV	the current value
DIFP.0	Num	The pre-exponential constant used in the calculation the component of the self-diffusivity due to diffusion with positive vacancies.	$microns^2$/ min.	the current value
DIFP.E	Num	The activation energy used in the calculation the component of the self-diffusivity due to diffusion with positive vacancies.	eV	the current value
DIFX.0	Num	The pre-exponential constant used in the calculation of the component of the self-diffusivity due to diffusion with neutral vacancies.	$microns^2$/ min.	the current value
DIFX.E	Num	The activation energy used in the calculation of the component of the self-diffusivity due to diffusion with neutral vacancies.	eV	the current value
DX.DEFAU	Num	The default nominal grid spacing for any layer containing this material.	microns	the current value
EPSILONF	Num	The dielectric constant of the material relative the dielectric constant of air.		the current value
GBE.0	Num	The pre-exponential constant used in calculating the grain-boundary energy		the current value
GBE.E	Num	The activation energy used in calculating the grain-boundary energy.	eV	the current value
GEO.FACT	Num	A geometric factor used in calculating the grain growth driving force, F.		the current value
GSZ.H.0	Num	The pre-exponential constant used in calculating the às deposited' polysilicon grain size for pressures near one atmosphere.	microns	the current value
GSZ.H.E	Num	The activation energy used in calculating the às deposited' polysilicon grain size for pressures near one atmosphere.	eV	the current value
GSZ.L.0	Num	The pre-exponential constant used in calculating the às deposited' polysilicon grain size for low pressure CVD.	microns	the current value
GSZ.L.E	Num	The activation energy used in calculating the `as deposited' polysilicon grain size for low pressure CVD.	eV	the current value
INDEX	Num	The material index of the material being modified. This number is used internally in the program to identify the material and point to its parameters.		
INSULATO	Log	Specifies that the material is an insulator.		false
K.M	Num	Used in R. Reif's epitaxial growth model (see reference in EPITAXY statement). K.m is the mass transport coefficient for silane in hydrogen.	microns/ min./atm	the current value
MIN.GRAI	Num	The minimum polysilicon grain size. Used for às deposited' LPCVD polysilicon when the temperature is below that specified by TEMP.BRE	microns	the current value

NAME	Char	The name of the material.		the current name of the material
NI.0	Num	The pre-factor used in the calculation of the intrinsic carrier concentration.	carriers/cm^3 (°K)$^{3/2}$	the current value
NI.E	Num	The activation energy used in the calculation of the intrinsic carrier concentration.	eV	the current value
NI.F	Num	The exponent to the absolute temperature used in the calculation of the intrinsic carrier concentration.		the current value
N.VALENC	Num	The carrier concentration in the valence band of the material.	carriers/cm^3	the current value
N.CONDUC	Num	The carrier concentration in the conduction band of the material.	carriers/cm^3	the current value
OEDK.0	Num	The pre-exponential constant used to calculate the relative contribution of oxidation enhanced diffusion to intrinsic diffusion.		the current value
OEDK.E	Num	The activation energy used to calculate the relative contribution of oxidation enhanced diffusion to intrinsic diffusion.	eV	the current value
OED.RATE	Num	The power dependence of oxidation enhanced diffusion on the oxidation rate.		the current value
RATIO.0	Num	The pre-exponential constant used to calculate the ratio of the silicon self-diffusivities in the grain and in the bulk. Actually the ratio of the pre-exponential factors for the two self-diffusivities		the current value
RATIO.E	Num	The activation energy used to calculate the ratio of the silicon self-diffusivities in the grain and in the bulk. Actually the difference between the activation energies of the two self-diffusivities	eV	the current value
SEMICOND	Log	Specifies that the material is a semiconductor.		false
SPECIES	Num	The number of different elements in this material.		the current value
TAU.0	Num	The pre-exponential constant used to calculate the time dependence of the grain interior concentration.	min.	the current value
TAU.E	Num	The activation energy used to calculate the time dependence of the grain interior concentration.	eV	the current value
TEMP.BRE	Num	For LPCVD the temperature below which the deposited polysilicon becomes amorphous.	°C	the current value
WORK.FUN	Num	The work function of the material.	V	the current value
100.OEDF	Num	The orientation dependent factor for the oxidation enhanced diffusion for <100> oriented silicon.		the current value
110.OEDF	Num	The orientation dependent factor for the oxidation enhanced diffusion for <110> oriented silicon.		the current value
111.OEDF	Num	The orientation dependent factor for the oxidation enhanced diffusion for <111> oriented silicon.		the current value

The MATERIAL statement is used to input or modify the coefficients and parameters that define a given material. Up to ten materials can be defined at one time. There are five default materials assigned the material indexes one through ten, these are single crystal silicon, silicon dioxide, polysilicon, silicon nitride, and aluminum. The first four of these should not be redefined as they are treated specially by several models in the program.

The current implementation of the program allows the definition of materials made up of at most three elements.

XXVI. Nitride Statement

The NITRIDE statement is used to input or modify the characteristics of silicon nitride as a layer material.

NITRIDE
[NAME=<c>] [DX.DEFAU=<n>] [INSULATO] [SPECIES=<n>] [DENSITY=<n>] [AT.WT.1=<n>] [AT.WT.2=<n>] [AT.NUM.1=<n>] [AT.NUM.2=<n>] [ABUND.1=<n>] [ABUND.2=<n>] [EPSILONF=<n>]

Name	Type	Description	Unit	Default
ABUND.1	Num	The relative abundance of element one in the material. The sum of all abundances for a material must equal one.		the current value
ABUND.2	Num	The relative abundance of element two in the material. The sum of all abundances for a material must equal one.		the current value
AT.NUM.1	Num	The atomic number of element one in the material.		the current value
AT.NUM.2	Num	The atomic number of element two in the material.		the current value
AT.WT.1	Num	The atomic weight of element one in the material.	amu	the current value
AT.WT.2	Num	The atomic weight of element two in the material.	amu	the current value
DENSITY	Num	The density of the material.	grams/cm^3	the current value
DX.DEFAU	Num	The default nominal grid spacing for any layer containing this material.	microns	the current value
EPSILONF	Num	The dielectric constant of the material relative the dielectric constant of air.		the current value
INSULATO	Log	Specifies that the material is an insulator.		false
NAME	Char	The name of the material.		the current name of the material
SPECIES	Num	The number of different elements in this material.		the current value

The NITRIDE statement is an alias for the MATERIAL statement with an index of four and is used to define or modify the parameters and coefficients associated with the material silicon nitride. Not all of the parameters of the MATERIAL statement apply to silicon nitride and so are not listed here.

XXVII. Nitrogen Statement

The NITROGEN statement allows the user to modify the coefficients used to model the oxidation of the various materials under nitrogen ambient or non-oxidizing conditions.

NITROGEN
[(<111> | <110> | <100>) [LIN.L.0=<n>] [LIN.L.E=<n>] [LIN.H.0=<n>] [LIN.H.E=<n>] [THINOX.0=<n>] [THINOX.E=<n>] [THINOX.L=<n>]] [PAR.L.0=<n>] [

PAR.L.E=<n>] [PAR.H.0=<n>] [PAR.H.E=<n>] [LIN.BREA=<n>] [PAR.BREA=<n>] [LIN.PDEP=<n>] [PAR.PDEP=<n>] [PRESSURE=<n>] [HCL%=<n>] [GAMMA.0=<n>] [GAMMA.E=<n>] [DELTA.0=<n>] [DELTA.E=<n>] [EXP.0=<n>] [EXP.E=<n>] [NIOX.0=<n>] [NIOX.E=<n>] [NIOX.F=<n>] [CL.ROW=<n> [CL.PCT=<n>] CL.COLUM=<n> [CL.TEMPE=<n>] [CL.DEP.L=<n>] [CL.DEP.P=<n>]]

Name	Type	Description	Unit	Default
CL.COLUM	Num	The column number in the table of coefficients used to calculate the chlorine dependence of the oxidation rates.		the current value
CL.DEP.L	Num	The coefficient modifying the linear oxidation rate in the presence of chlorine at the specified row and column.		the current value
CL.DEP.P	Num	The coefficient modifying the parabolic oxidation rate in the presence of chlorine at the specified row and column.		the current value
CL.PCT	Num	The percentage of chlorine for which the coefficients in the specified row are valid.	percent	the current value
CL.ROW	Num	The row number in the table of coefficients used to calculate the chlorine dependence of the oxidation rates.		the current value
CL.TEMPE	Num	The temperature for which the coefficients in the specified column are valid.	°C	the current value
DELTA.0	Num	The pre-exponential factor of the delta coefficient used in calculating the impurity concentration dependence of the parabolic oxidation rate.	cm^3/atom	the current value
DELTA.E	Num	The activation energy of the delta coefficient used in calculating the impurity concentration dependence of the parabolic oxidation rate.	eV	the current value
EXP.0	Num	The pre-exponential factor of the exponent used in calculating the impurity concentration dependence of the parabolic oxidation rate.		the current value
EXP.E	Num	The activation energy of the exponent used in calculating the impurity concentration dependence of the parabolic oxidation rate.	eV	the current value
GAMMA.0	Num	The pre-exponential factor of the gamma coefficient used in calculating the impurity concentration dependence of the linear oxidation rate.		the current value
GAMMA.E	Num	The activation energy of the gamma coefficient used in calculating the impurity concentration dependence of the linear oxidation rate.	eV	the current value
HCL%	Num	The default percentage of chlorine present in the ambient.	percent	the current value
LIN.BREA	Num	The temperature at which the temperature dependence of the linear oxidation rate changes.	°C	the current value
LIN.H.0	Num	The pre-exponential constant of the linear oxidation rate for temperatures above the breakpoint set by L.BREAKP.	microns/ min.	the current value
LIN.H.E	Num	The activation energy of the linear oxidation rate for temperatures above the breakpoint set by L.BREAKP.	eV	the current value

LIN.L.0	Num	The pre-exponential constant of the linear oxidation rate for temperatures below the breakpoint set by L.BREAKP.	microns/ min.	the current value
LIN.L.E	Num	The activation energy of the linear oxidation rate for temperatures below the breakpoint set by L.BREAKP.	eV	the current value
LIN.PDEP	Num	The pressure dependence factor for the linear oxidation rate.		the current value
NIOX.0	Num	The pre-exponential constant used to determine the oxidation rate of silicon nitride.	microns	the current value
NIOX.E	Num	The activation energy used to determine the oxidation rate of silicon nitride.	eV	the current value
NIOX.F	Num	The exponent factor used to determine the oxidation rate of silicon nitride.		the current value
PAR.BREA	Num	The temperature at which the temperature dependence of the parabolic oxidation rate changes.	°C	the current value.
PAR.H.0	Num	The pre-exponential constant of the parabolic oxidation rate for temperatures above the breakpoint set by P.BREAKP.	$microns^2$/ min.	the current value
PAR.H.E	Num	The activation energy of the parabolic oxidation rate for temperatures above the breakpoint set by P.BREAKP.	eV	the current value
PAR.L.0	Num	The pre-exponential constant of the parabolic oxidation rate for temperatures below the breakpoint set byP.BREAKP.	$microns^2$/ min.	the current value
PAR.L.E	Num	The activation energy of the parabolic oxidation rate for temperatures below the breakpoint set by P.BREAKP.	eV	the current value
PAR.PDEP	Num	The pressure dependence factor for the parabolic oxidation rate.		the current value
PRESSURE	Num	The default ambient pressure.	atm.	the current value
THINOX.0	Num	The pre-exponential constant of the thin oxide growth rate parameter.	microns/ min.	the current value
THINOX.E	Num	The activation energy of the thin oxide growth rate parameter.	eV)	the current value
THINOX.L	Num	The characteristic length of the thin oxide growth rate parameter.	microns	the current value
<100>	Log	Specifies that the linear growth rate and thin oxide growth rate parameters apply to <100> orientation silicon.		false
<110>	Log	Specifies that the linear growth rate and thin oxide growth rate parameters apply to <110> orientation silicon.		false
<111>	Log	Specifies that the linear growth rate and thin oxide growth rate parameters apply to <111> orientation silicon.		false

The three oxidation model statements, DRYO2, WETO2, and NITROGEN, use identical parameters, differing only in the values assigned. The parameters NIOX.C, NIOX.E, and NIOX.F are used in modeling the oxidation of silicon nitride while the others deal with the oxidation of single and polycrystalline silicon.

The effects of chlorine in the ambient gas on the oxidation rate of silicon are currently modeled by an empirical expression whose only variable is defined by the L.CLDEP and P.CLDEP for the linear and parabolic rates respectively. To date no convenient function is available to calculate the chlorine dependence as a function of temperature and amount of chlorine present, therefor a table of values defines the chlorine dependence factors at those temperatures and percentages for which reliable data is available. For those temperatures and chlorine percentages between the values in the table, linear interpolation is employed to calculate the value used. For temperatures or percentages outside the range of values present in the table, the values whose conditions most nearly match the current conditions are used. For example, if the current conditions are a temperature of 1175 degrees with three percent chlorine, but the highest temperature entry in the table is 1150 degrees and the nearest chlorine percentages are for two and four percent, then a value halfway between the values at 1150 degrees and two and four percent chlorine will be used.

XXVIII.Oxide Statement

The OXIDE statement is used to input or modify the characteristics of silicon dioxide as a layer material.

OXIDE
[NAME=<c>] [DX.DEFAU=<n>] [INSULATO] [SPECIES=<n>] [DENSITY=<n>] [AT.WT.1=<n>] [AT.WT.2=<n>] [AT.NUM.1=<n>] [AT.NUM.2=<n>] [ABUND.1=<n>] [ABUND.2=<n>] [EPSILONF=<n>]

Name	Type	Description	Unit	Default
ABUND.1	Num	The relative abundance of element one in the material. The sum of all abundances for a material must equal one.		the current value
ABUND.2	Num	The relative abundance of element two in the material. The sum of all abundances for a material must equal one.		the current value
AT.NUM.1	Num	The atomic number of element one in the material.		the current value
AT.NUM.2	Num	The atomic number of element two in the material.		the current value
AT.WT.1	Num	The atomic weight of element one in the material.	amu	the current value
AT.WT.2	Num	The atomic weight of element two in the material.	amu	the current value
DENSITY	Num	The density of the material.	grams/cm^3	the current value
DX.DEFAU	Num	The default nominal grid spacing for any layer containing this material.	microns	the current value
EPSILONF	Num	The dielectric constant of the material relative the dielectric constant of air.		the current value
INSULATO	Log	Specifies that the material is an insulator.		false
NAME	Char	The name of the material.		the current name of the material
SPECIES	Num	The number of different elements in this material.		the current value

The OXIDE statement is an alias for the MATERIAL statement with an index of two and is used to define or modify the parameters and coefficients associated with the material silicon dioxide. Not all of the parameters of the MATERIAL statement apply to silicon dioxide and so are not listed here.

XXIX. Phosphorus Statement

The PHOSPHOR statement is used to input or modify the physical or model coefficients associated with phosphorus as a dopant impurity.

PHOSPHOR
[NAME=<c>] [DONOR] [AT.WT=<n>] [AT.NUMB=<n>] [IONFILE1=<c>] [IONFILE2=<c>]
[((SILICON [FII.0=<n>] [FII.E=<n>] [K.MF=<n>] [K.A=<n>] [K.P=<n>] [MISFITST=<n>] [CD=<n>] [MSF111FA=<n>] [MSF110FA=<n>] [MSF100FA=<n>] [DAMAGEST=<n>] [NE.0=<n>] [NE.E=<n>] [(IMPLANT | CHEMICAL) [CTN.0=<n>] [CTN.E=<n>] [CTN.F=<n>]]) | (POLYSILI [ENTROPY=<n>] [HEAT.SEG=<n>] [Q.SITES=<n>] [FII.0=<n>] [FII.E=<n>] [(IMPLANT | CHEMICAL) [CTN.0=<n>] [CTN.E=<n>] [CTN.F=<n>]]) | (OXIDE | NITRIDE | ALUMINUM)
[ELECT.ST=<n>] [DIX.0=<n>] [DIX.E=<n>] [DIM.0=<n>] [DIM.E=<n>] [DIMM.0=<n>] [DIMM.E=<n>]]

Name	Type	Description	Unit	Default
ALUMINUM	Log	Specifies that the material dependent parameters apply to phosphorus in aluminum.		false
AT.NUMB	Num	The atomic number of the impurity.		the current value
AT.WT	Num	The atomic weight of the impurity.	amu	the current value
CD	Num	This parameter is used to calculate the temperature dependent part of the expression for bandgap narrowing due to lattice misfit strain from high concentrations of phosphorus.	(atoms/cm^3)(°C^2)	the current value
CHEMICAL	Log	Specifies that the clustering coefficients apply to the impurity from a chemical source.		false
CTN.0	Num	The pre-exponential constant used in calculating the impurity clustering coefficient.	atoms/cm^3	the current value
CTN.E	Num	The activation energy used in calculating the impurity clustering coefficient.	eV	the current value
CTN.F	Num	The power dependence of the concentration used in calculating the impurity clustering coefficient.		the current value
DAMAGEST	Num	The factor in the implant dose dependent expression for calculating the bandgap narrowing due to the residual damage of phosphorus implants.	eV cm$^{1/2}$	the current value
DIM.0	Num	The pre-exponential constant of the diffusion coefficient of the impurity diffusing with singly negative vacancies.	microns^2/min.	the current value
DIM.E	Num	The activation energy of the diffusion coefficient of the impurity diffusing with singly negative vacancies.	eV	the current value
DIMM.0	Num	The pre-exponential constant of the diffusion coefficient of the impurity diffusing with doubly negative vacancies.	microns^2/min.	the current value
DIMM.E	Num	The activation energy of the diffusion coefficient of the impurity diffusing with doubly negative vacancies.	eV	the current value
DIX.0	Num	The pre-exponential constant of the diffusion coefficient of the impurity diffusing with neutral vacancies.	microns^2/min.	the current value
DIX.E	Num	The activation energy of the diffusion coefficient	eV	the current value

		of the impurity diffusing with neutral vacancies.		
DONOR	Log	Specifies that the impurity is a donor in silicon.		the current value
ELECT.ST	Num	The electric stopping power of the impurity in the specified material.	KeV/micron.	the current value
ENTROPY	Num	The entropy factor. Used to calculate the equilibrium segregation factor at polysilicon grain boundaries.		the current value
FII.0	Num	The pre-exponential constant of the fractional partial-interstitialcy contribution.	$(\text{microns/min.})^{-1/2}$	the current value
FII.E	Num	The activation energy of the fractional partial-interstitialcy contribution.	eV	the current value
HEAT.SEG	Num	The activation energy of the equilibrium segregation factor at polysilicon grain boundaries.	eV	the current value
IMPLANT	Log	Specifies that the impurity clustering coefficients apply to the impurity from an implanted source.		false
IONFILE1	Char	Specifies the primary ion implant range data file for implants using the analytic distributions. This file will be searched for the range statistics when implanting atomic phosphorus.		the last file specified
IONFILE2	Char	Specifies the secondary ion implant range data file for implants using the analytic distributions. This file will be searched for the range statistics when implanting the compound ions containing phosphorus.		the last file specified
K.A	Num	Used in R. Reif's epitaxial doping model (see reference in EPITAXY statement). K.a is a thermodynamic constant relating the dopant species concentration in solid silicon and adsorbed layer.	cm	the current value
K.MF	Num	Used in R. Reif's epitaxial doping model (see reference in EPITAXY statement). K.mf is a kinetic coefficient controlling the rate-limiting step of the dopant incorporation process.	cm^{-2} min^{-1} atm^{-1}	the current value
K.P	Num	Used in R. Reif's epitaxial doping model (see reference in EPITAXY statement). K.p is a thermodynamic constant relating the dopant species concentration in solid silicon and gas phase.	cm^{-3} atm^{-1}	the current value
MISFITST	Num	The prefactor in the high concentration dependent expression for calculating the bandgap narrowing due to the lattice misfit strain from high concentrations of phosphorus.	$eV\text{-}cm^3$	the current value
MSF100FA	Num	The orientation factor in <100> orientation silicon for bandgap narrowing due to lattice misfit strain from high concentrations of phosphorus.		the current value
MSF110FA	Num	The orientation factor in <110> orientation silicon for bandgap narrowing due to lattice misfit strain from high concentrations of phosphorus.		the current value
MSF111FA	Num	The orientation factor in <111> orientation silicon for bandgap narrowing due to lattice misfit strain from high concentrations of phosphorus.		the current value

NAME	Char	The name of the impurity.		the last name specified
NE.0	Num	The pre-exponential constant for Ne, the concentration at which the P+V= pairs disassociate. Used to calculate the diffusivity of phosphorus at high concentrations.	atoms/cm^3	the current value
NE.E	Num	The activation energy for calculating Ne, the concentration at which the P+V= pairs disassociate. Used to calculate the diffusivity of phosphorus at high concentrations.	eV	the current value
NITRIDE	Log	Specifies that the material dependent parameters apply to phosphorus in silicon nitride.		false
OXIDE	Log	Specifies that the material dependent parameters apply to phosphorus in silicon dioxide.		false
POLYSILI	Log	Specifies that the material dependent parameters apply to phosphorus in polysilicon.		false
Q.SITES	Num	Effective density of segregation sites at a grain boundary.	sites/cm^2	the current value
SILICON	Log	Specifies that the material dependent parameters apply to phosphorus in silicon.		false

The PHOSPHOR statement is an alias for the IMPURITY statement with an index of two and is used to define or modify the parameters and coefficients associated with phosphorus as an impurity. Not all of the parameters of the IMPURITY statement apply to phosphorus and so are not listed here.

XXX. Plot Statement

The PLOT statement outputs a semi-Logarithmic plot of the specified impurity concentrations versus depth into the structure.

PLOT
[ACTIVE] [CHEMICAL] [TOTAL] [NET] [ANTIMONY] [ARSENIC] [BORON] [PHOSPHOR] [XMIN=<n>] [XMAX=<n>] [CMIN=<n>] [CMAX=<n>]
[((HP2648A | HP2623A) [CLEAR] [AXIS] [XPWIDTH=<n>] [YPWIDTH=<n>] [XPTS.IN=<n>] [YPTS.IN=<n>] [XOFSET=<n>] [YOFSET=<n>]] [LINETYPE=<n>] [FILENAME=<c>]) | (LP.PLOT [LINES/PA=<n>] [COLUMNS=<n>])]

Name	Type	Description	Unit	Default	Synonym
ACTIVE	Log	Specifies that the electrically active concentrations of the specified impurities are to be plotted.		false	
ANTIMONY	Log	Specifies that the antimony concentration, either active and/or chemical, is to be plotted.		false	SB
ARSENIC	Log	Specifies that the arsenic concentration, either active and/or chemical, is to be plotted.		false	AS
AXIS	Log	Specifies that the axis is to be plotted. Not used by line printer plots.		true	
BORON	Log	Specifies that the boron concentration, either active and/or chemical, is to be plotted.		false	
CHEMICAL	Log	Specifies that the chemical concentration of the specified impurities are to be plotted.		false	

CLEAR	Log	Causes the plot area to be cleared. Not used by line printer plots.		true	
COLUMNS	Num	The number of columns to be used in line printer plots.	columns	80	
CMAX	Num	The maximum concentration value plotted.	atoms/cm^3	$1x10^{21}$	
CMIN	Num	The minimum concentration value plotted.	atoms/cm^3	$1x10^{14}$	
FILENAME	Char	Specifies a file to receive the x, y and pen control parameters.			
HP2623A	Log	Specifies that the plot device is a Hewlett-Packard 2623A graphics terminal, or equivalent.		false	2623A
HP2648A	Log	Specifies that the plot device is a Hewlett-Packard 2648A graphics terminal, or equivalent.		false	2648A
LINETYPE	Num	Sets the line type used when plotting the impurity distribution. A solid line and various dotted and dashed line types are available.		1 i.e. solid line	
LINES/PA	Num	The number of lines to be used in plots to the line printer.	lines/page	60	
LP.PLOT	Log	Specifies that the plot output is output to the standard output device, usually a line printer.		false	LPPLOT
NET	Log	Specifies that the difference of the sum of the n-type and the sum p-type active or chemical impurity concentrations present in the structure is to be plotted.		false	
PHOSPHOR	Log	Specifies that the phosphorus concentration, either active and/or chemical, is to be plotted.		false	
TOTAL	Log	Specifies that the sum of the active or chemical impurity concentrations present in the structure is to be plotted.		false	
XMAX	Num	The distance from the top of the structure to the point where the last concentration is to be plotted.	microns	The current depth of the structure	
XMIN	Num	The distance from the top of the structure to the point where the first concentration is to be plotted.	microns	0.0	
XOFFSET	Num	The distance that the plot is to be offset from the origin of the plot device in the x direction.	inches	0.5	
XPTS.IN	Num	The number of plot points per inch in the x direction.	points/inch	72 for hp2648, 60 for hp 2623	
XPWIDTH	Num	The plot width (x direction).	inches	8.0 for hp2648, 8.5 for hp 2623	
YOFSET	Num	The distance that the plot is to be offset from the origin of the plot device in the y direction.	inches	1.0	
YPTS.IN	Num	The number of plot points per inch in the y direction.	points/inch	72 for hp2648, 60 for hp	

YPWIDTH	Num	The plot height (y direction).	inches	2623 4.0 for hp2638, 6 for hp 2623

The PLOT statement is used to output plots of the impurity distributions versus distance in the structure. A number of plot devices are available, line printer and any of the Hewlett-Packard 26xx graphics terminals.

The impurities present may be plotted either individually, added together, or as the difference between n- and p-type dopants. These plots may be of either the electrically active or total chemical concentrations.

If no range is specified, then the distributions are plotted over the entire structure. If no minimum or maximum plot concentrations are specified, then the range between $1x10^{14}$ and $1x10^{21}$ is plotted.

XXXI. Polysilicon Statement

The POLYSILI statement is used to input or modify the characteristics of polycrystalline silicon as a layer material.

POLYSILI
[NAME=<c>] [DX.DEFAU=<n>] [SEMICOND] [SPECIES=<n>] [DENSITY=<n>] [AT.WT.1=<n>] [AT.NUM.1=<n>] [ABUND.1=<n>] [DIFX.0=<n>] [DIFX.E=<n>] [DIMX.0=<n>] [DIFM.E=<n>] [DIMMX.0=<n>] [DIFMM.E=<n>] [DIFP.0=<n>] [DIFP.E=<n>] [NI.0=<n>] [NI.E=<n>] [NI.F=<n>] [DEFECTLN=<n>] [OEDK.0=<n>] [OEDK.E=<n>] [OED.RATE=<n>] [GSZ.H.0=<n>] [GSZ.H.E=<n>] [GSZ.L.0=<n>] [GSZ.L.E=<n>] [MIN.GRAI=<n>] [TEMP.BRE=<n>] [RATIO.0=<n>] [RATIO.E=<n>] [GEO.FACT=<n>] [GBE.0=<n>] [GBE.E=<n>] [TAU.0=<n>] [TAU.E=<n>] [AFFINITY=<n>] [EPSILONF=<n>] [N.VALENC=<n>] [N.CONDUC=<n>] [BAND.GAP=<n>]

Name	Type	Description	Unit	Default
ABUND.1	Num	The relative abundance of element one in the material. The sum of all abundances for a material must equal one.		the current value
AFFINITY	Num	The electron affinity of the material.	eV	the current value
AT.NUM.1	Num	The atomic number of element one in the material.		the current value
AT.WT.1	Num	The atomic weight of element one in the material.	amu	the current value
BAND.GAP	Num	The band gap of the material.	eV	the current value
DEFECTLN	Num	The decay length of point defects in the material.	microns	the current value
DENSITY	Num	The density of the material.	grams/cm^3	the current value
DIFM.0	Num	The pre-exponential constant used in the calculation the component of the self-diffusivity due to diffusion with singly negative vacancies.	microns^2/min	the current value
DIFM.E	Num	The activation energy used in the calculation the component of the self-diffusivity due to diffusion with singly negative vacancies.	eV	the current value
DIFMM.0	Num	The pre-exponential constant used in the calculation of the component of the self-diffusivity due to diffusion with doubly negative	microns^2/min.	the current value

		vacancies.		
DIFMM.0	Num	The activation energy used in the calculation the component of the self-diffusivity due to diffusion with doubly negative vacancies.	eV	the current value
DIFP.0	Num	The pre-exponential constant used in the calculation the component of the self-diffusivity due to diffusion with positive vacancies.	$microns^2$/min.	the current value
DIFP.E	Num	The activation energy used in the calculation the component of the self-diffusivity due to diffusion with positive vacancies.	eV	the current value
DIFX.0	Num	The pre-exponential constant used in the calculation of the component of the self-diffusivity due to diffusion with neutral vacancies.	$microns^2$/min.	the current value
DIFX.E	Num	The activation energy used in the calculation of the component of the self-diffusivity due to diffusion with neutral vacancies.	eV	the current value
DX.DEFAU	Num	The default nominal grid spacing for any layer containing this material.	microns	the current value
EPSILONF	Num	The dielectric constant of the material relative the dielectric constant of air.		the current value
GBE.0	Num	The pre-exponential constant used in calculating the grain-boundary energy		the current value
GBE.E	Num	The activation energy used in calculating the grain-boundary energy.	eV	the current value
GEO.FACT	Num	A geometric factor used in calculating the grain growth driving force, F.		the current value
GSZ.H.0	Num	The pre-exponential constant used in calculating the às deposited' polysilicon grain size for pressures near one atmosphere.	microns	the current value
GSZ.H.E	Num	The activation energy used in calculating the às deposited' polysilicon grain size for pressures near one atmosphere.	eV	the current value
GSZ.L.0	Num	The pre-exponential constant used in calculating the às deposited' polysilicon grain size for low pressure CVD.	microns	the current value
GSZ.L.E	Num	The activation energy used in calculating the às deposited' polysilicon grain size for low pressure CVD.	eV	the current value
MIN.GRAI	Num	The minimum polysilicon grain size. Used for às deposited' LPCVD polysilicon when the temperature is below that specified by TEMP.BRE	microns	the current value
NAME	Char	The name of the material.		the current name of the material
NI.0	Num	The pre-factor used in the calculation of the intrinsic carrier concentration.	(carriers/cm^3)$(°K)^{3/2}$	the current value
NI.E	Num	The activation energy used in the calculation of the intrinsic carrier concentration.	eV	the current value
NI.F	Num	The exponent to the absolute temperature used in the calculation of the intrinsic carrier concentration.		the current value

N.CONDUC	Num	The carrier concentration in the conduction band of the material.	carriers/cm^3	the current value
N.VALENC	Num	The carrier concentration in the valence band of the material.	carriers/cm^3	the current value
OEDK.0	Num	The pre-exponential constant used to calculate the relative contribution of oxidation enhanced diffusion to intrinsic diffusion.		the current value
OEDK.E	Num	The activation energy used to calculate the relative contribution of oxidation enhanced diffusion to intrinsic diffusion.	eV	the current value
OED.RATE	Num	The power dependence of oxidation enhanced diffusion on the oxidation rate.		the current value
RATIO.0	Num	The pre-exponential constant used to calculate the ratio of the silicon self-diffusivities in the grain and in the bulk. Actually the ratio of the pre-exponential factors for the two self-diffusivities		the current value
RATIO.E	Num	The activation energy used to calculate the ratio of the silicon self-diffusivities in the grain and in the bulk. Actually the difference between the activation energies of the two self-diffusivities	eV	the current value
SEMICOND	Log	Specifies that the material is a semiconductor.		false
SPECIES	Num	The number of different elements in this material.		the current value
TAU.0	Num	The pre-exponential constant used to calculate the time dependence of the grain interior concentration.	min.	the current value
TAU.E	Num	The activation energy used to calculate the time dependence of the grain interior concentration.	eV	the current value
TEMP.BRE	Num	For LPCVD the temperature below which the deposited polysilicon becomes amorphous.	°C	the current value

The POLYSILI statement is an alias for the MATERIAL statement with an index of three and is used to define or modify the parameters and coefficients associated with the material polysilicon. Not all of the parameters of the MATERIAL statement apply to polysilicon and so are not listed here.

XXXII.Print Statement

The PRINT statement outputs information about the structure being simulated and the coefficients used in the simulation. The printed out-put may consist of the impurity concentrations versus depth into the structure, junction depths, sheet resistivities, layer thicknesses, diffusion or oxidation rates, etc.

PRINT
[CONCENTR [ACTIVE] [CHEMICAL] [ALL] [TOTAL] [NET] [ANTIMONY] [ARSENIC] [BORON] [PHOSPHOR] [XMIN=<n>] [XMAX=<n>]] [IMPURITY [ALL | (ANTIMONY | ARSENIC | BORON | PHOSPHOR)]]
[MATERIAL [ALL | (SILICON | POLYSILI | OXIDE | NITRIDE | ALUMINUM)]]
[LAYERS] [SEGREGAT] [OXIDATIO] [LINES/PA=<n>] [COLUMNS=<n>] [LU=<n> | FILENAME=<c>]

Name	Type	Description	Unit	Default	Synonym
ACTIVE	Log	Specifies that the electrically active concentration of the specified impurities are to be printed.		false	

ALL	Log	Specifies that the impurity coefficient information for all impurities is to be printed, or that the impurity distributions of all impurities present in the structure are to be printed.		false	
ALUMINUM	Log	Specifies that the material coefficient information for aluminum is to be printed.		false	
ANTIMONY	Log	Specifies that the antimony concentration, either active or chemical, is to be printed, or that the antimony coefficient information is to be printed.		false	SB
ARSENIC	Log	Specifies that the arsenic concentration, either active or chemical, is to be printed, or that the arsenic coefficient information is to be printed.		false	AS
BORON	Log	Specifies that the boron concentration, either active or chemical, is to be printed, or that the boron coefficient information is to be printed.		false	
CHEMICAL	Log	Specifies that the chemical concentration of the specified impurities are to be printed.	false		
COLUMNS	Num	The number of columns to be used in the printed out-put.	columns	80	
CONCENTR	Log	Causes the specified impurity concentrations versus depth to be printed.		false	
FILENAME	Char	The name of a file to which the information is to be output.			
IMPURITY	Log	Specifies that the coefficient information concerning the specified impurities is to be printed (e.g. diffusion coefficients, atomic number and mass, etc.)		false	
LAYERS	Log	Specifies that information concerning the layers of the current structure is to be printed (e.g. layer thickness, junction depths, integrated dopant concentrations, etc.)		false	
LINES/PA	Num	The number of lines per page in the printed output.	lines/page	60	
LU	Num	The Logical unit number to which the information is to be output.		the standard output lu	
MATERIAL	Log	Specifies that the coefficient information concerning the specified materials is to be printed (e.g. band gap, intrinsic carrier concentration coefficients, electric stopping powers, etc.)		false	
NET	Log	Specifies that the sum of the n-type minus the sum of the p-type active or chemical impurity concentrations are to be printed.		false	
NITRIDE	Log	Specifies that the material coefficient information for silicon nitride is to be printed.		false	
OXIDATIO	Log	Specifies that the coefficients that determine the oxidation of silicon, polysilicon and silicon nitride are to be printed.		false	
OXIDE	Log	Specifies that the material coefficient information for silicon dioxide is to be printed.		false	
PHOSPHOR	Log	Specifies that the phosphorus concentration, either active or chemical, is to be printed, or that		false	

		the phosphorus coefficient information is to be printed.		
POLYSILI	Log	Specifies that the material coefficient information for polysilicon is to be printed.		false
SEGREGAT	Log	Specifies that the coefficients that determine the segregation of impurities across material interfaces are to be printed. The mass transport coefficients and the volume ratios are also printed.		false
SILICON	Log	Specifies that the material coefficient information for single crystal silicon is to be printed.		false
TOTAL	Log	Specifies that the sum of all of the active or chemical impurity concentrations present in the structure is to be printed.		false
XMAX	Num	The distance from the top of the structure to the point where the last concentration is to be printed.	microns	The current depth of the structure
XMIN	Num	The distance from the top of the structure to the point where the first concentration is to be printed.	microns	0.0

The PRINT statement is used to output printed information. This information may consist of structural information such as junction depths, layer thicknesses or various impurity distributions versus distance in the structure, or coefficient information such as the coefficients for impurity diffusion or segregation, the oxidation of silicon, or the atomic number and mass of impurities or materials.

The impurities present may be printed either individually, added together, or as the difference between n- and p-type dopants. These prints may be of either electrically or total chemical concentrations.

If no range is specified, then the distributions are printed over the entire structure.

Normally the output of the print statement goes to the standard output device (usually the line printer), but the user may override the output Logical unit number by specifying the output lu, or he may direct it into a specified file.

XXXIII.Profile Statement

The PROFILE statement is used to input an arbitrary impurity profile from a data file. The data must be stored as two columns, one being the distance from the origin and the other being the concentration at that point.

PROFILE
FILE=<c> CONC.COL=<n> X.COL=<n> [LAYER=<n>] [SKIP=<n>] [COUNT=<n>] [COM.CHAR=<c>] (ANTIMONY | ARSENIC | BORON | PHOSPHOR)

Name	Type	Description	Default	Synonym
ANTIMONY	Log	Specifies that the profile data is for the dopant antimony.	false	SB
ARSENIC	Log	Specifies that the profile data is for the dopant arsenic.	false	AS
BORON	Log	Specifies that the profile data is for the dopant boron.	false	
COM.CHAR	Char	Specifies the comment character for the lines in the file. Any line with this character in column one is ignored.	*	
CONC.COL	Num	Specifies the column in the file containing the concentration data.		

COUNT	Num	Specifies the number of data points to be input.	Input all every data point.
LAYER	Num	Specifies the layer at which the first data point is to be placed.	Topmost layer
PHOSPHOR	Log	Specifies that the profile data is for the dopant phosphorus.	false
SKIP	Num	Specifies the number of data points to be skipped on input.	0
X.COL	Num	Specifies the column in the file containing the distance of each data point from the origin.	

The PROFILE statement inputs an arbitrary impurity distribution of the specified dopant from a data file. The data files must be organized in columns, with one column containing the concentration data and another containing the distance from the origin at which the corresponding concentration applies. The data in the columns must be organized such that the locations are in increasing order. Comment lines may appear at any point as long as they are preceded the comment character in column one.

XXXIV.Resistivity Statement

The RESISTIVITY statement is used to input a table of ordered resistivity/concentration pairs. This data is used by the program to calculate the resistivity of diffused layers in the current structure.

RESISTIVITY
FILE=<c> CONC.COL=<n> RES.COL=<n> [SKIP=<n>] [COUNT=<n>] [COM.CHAR=<c>] (ANTIMONY | ARSENIC | BORON | PHOSPHOR) (ALUMINUM | NITRIDE | OXIDE | POLYSILICON | SILICON)

Name	Type	Description	Default	Synonym
ALUMINUM	Log	Specifies that the resistivity data applies to the impurity in the material aluminum.	false	
ANTIMONY	Log	Specifies that the resistivity data applies to the dopant antimony.	false	SB
ARSENIC	Log	Specifies that the resistivity data applies to the dopant arsenic.	false	AS
BORON	Log	Specifies that the resistivity data applies to the dopant boron.	false	
COM.CHAR	Char	Specifies the comment character for the lines in the file. Any line with this character in column one is ignored.	*	
CONC.COL	Num	Specifies the column in the data file containing the concentrations at which the resistivity data applies.		CON.COL
COUNT	Num	Specifies the number of data points to be input.	Input all every data point	
NITRIDE	Log	Specifies that the resistivity data applies to the impurity in the material nitride.	false	
OXIDE	Log	Specifies that the resistivity data applies to the impurity in the material oxide.	false	
PHOSPHOR	Log	Specifies that the resistivity data applies to the dopant phosphorus.	false	
POLYSILI	Log	Specifies that the resistivity data applies to the impurity in the material polysilicon.	false	

RES.COL	Num	Specifies the column in the data file containing the resistivities associated with the corresponding concentration values.	
SKIP	Num	Specifies the number of data points to be skipped on input.	0
SILICON	Log	Specifies that the resistivity data applies to the impurity in the material silicon.	false

The RESISTIVITY statement inputs the resistivity vs. concentration data from the specified file and associates it with one or more impurities in one or more materials. The data files must be organized in columns, with one column containing the resistivity values and another containing corresponding impurity concentrations. The data in the columns must be organized such that the concentration values are in increasing order. Comment lines may appear at any point as long as they are preceded with the comment character in column one.

XXXV.Savefile Statement

The SAVEFILE statement is used to save either the current structure being processed, the physical and model coefficients being used, or both.

SAVEFILE
FILENAME=<c> (ALL | COEFFICI | STRUCTUR | EXPORT)

Name	Type	Description	Default	Synonym
ALL	Log	Specifies that both the structure information and the model coefficients are to be written to the specified file.	false	
COEFFICI	Log	Specifies that the coefficient information is to be written to the specified file.	false	
EXPORT	Log	Specifies that the structure information be written in export format for use by a post-processor or device simulation program such as SEDAN-II or PISCES-II	false	
FILENAME	Char	The name of the file to which the specified information is to be written.		NAME
STRUCTUR	Log	Specifies that the information describing the current structure is to be written to the specified file.	false	

The SAVEFILE statement saves two classes of information. One is class contains all of the physical and model parameters or coefficients used by the program. A file containing this information is used by the INITIALIZATION statement at the beginning of each processing sequence to initialize the program. The other class of information contains the physical structure and impurity distributions of the materials being simulated. There are two types of files that can be written containing this class of information. One, the structure file, may be used as the starting point for subsequent processing simulations in order to model process run splits or examine process sensitivity. The other is the export file which stores the current structure information in a format that is designed to be read by either post-processors or device simulation programs such as SEDAN-II or PISCES-II.

The information stored by the SAVEFILE statement, except for export files, can be read into the program either by the INITIALIZE statement at the start of a process, or at any time by a LOADFILE statement.

XXXVI.Segregation Statement

The SEGREGAT statement is used to define or modify the impurity segregation coefficient and the impurity transport coefficient across the interface between two material layers.

SEGREGAT

((SILICON [100.FACT=<n>] [110.FACT=<n>] [111.FACT=<n>]) | OXIDE | POLYSILI | NITRIDE | ALUMINUM | AIR)
((/SILICON [100.FACT=<n>] [110.FACT=<n>] [111.FACT=<n>]) | /OXIDE | /POLYSIL | /NITRIDE | /ALUMINU | /AIR)
(ANTIMONY | ARSENIC | BORON | PHOSPHOR) [SEG.0=<n>] [SEG.E=<n>] [TRANS.0=<n>] [TRANS.E=<n>] [MUI.0=<n>] [MUI.E=<n>]

Name	Type	Description	Unit	Default	Synonym
AIR	Log	Specifies that the material above the interface is the ambient gas.		False	AMBIENT
ALUMINUM	Log	Specifies that the material above the interface is aluminum.		False	
ANTIMONY	Log	Specifies that the coefficients apply to the dopant antimony.		false	
ARSENIC	Log	Specifies that the coefficients apply to the dopant arsenic.		false	
BORON	Log	Specifies that the coefficients apply to the dopant boron.		false	
MUI.0	Num	The pre-exponential factor for the chemical potential segregation term.	microns	the current value	
MUI.E	Num	The activation energy for the chemical potential segregation term.	eV	the current value	
NITRIDE	Log	Specifies that the material above the interface is silicon nitride.		false	
OXIDE	Log	Specifies that the material above the interface is silicon dioxide.		false	
PHOSPHOR	Log	Specifies that the specified coefficients apply to the dopant phosphorus.		false	
POLYSILI	Log	Specifies that the material above the interface is polysilicon.		false	
SEG.0	Num	The pre-exponential factor of the segregation coefficient.		the current value	
SEG.E	Num	The activation energy of the segregation coefficient.	eV	the current value	
SILICON	Log	Specifies that the material above the interface is single crystal silicon.	false		
TRANS.0	Num	The pre-exponential factor of the interface transport coefficient.	microns/ min.	the current value	
TRANS.E	Num	The activation energy of the interface transport coefficient.	eV	the current value	
/AIR	Log	Specifies that the material below the interface is air.		false	AMBIENT
/ALUMINU	Log	Specifies that the material below the interface is aluminum.		false	
/NITRIDE	Log	Specifies that the material below the		false	

		interface is silicon nitride.	
/OXIDE	Log	Specifies that the material below the interface is silicon dioxide.	false
/POLYSIL	Log	Specifies that the material below the interface is polysilicon.	false
/SILICON	Log	Specifies that the material below the interface is single crystal silicon.	false
100.FACT	Num	The orientation factor of the impurity's segregation coefficient for <100> orientation silicon.	the current value
110.FACT	Num	The orientation factor of the impurity's segregation coefficient for <110> orientation silicon.	the current value
111.FACT	Num	The orientation factor of the impurity's segregation coefficient for <111> orientation silicon.	the current value

The SEGREGAT statement defines those parameters that have to do with transport of impurities across material interfaces. The impurity type must be specified as well as the the material types on either side of the interface. The material above the interface is specified simply by name, while the material below the interface is specified by its name preceded by a slash `/'.

XXXVII.Silicon Statement

The SILICON statement is used to input or modify the characteristics of single crystal silicon as a layer material.

SILICON
[NAME=<c>] [DX.DEFAU=<n>] [SEMICOND] [SPECIES=<n>] [DENSITY=<n>] [AT.WT.1=<n>] [AT.NUM.1=<n>] [ABUND.1=<n>] [NI.0=<n>] [NI.E=<n>] [NI.F=<n>] [DEFECTLN=<n>] [OEDK.0=<n>] [OEDK.E=<n>] [OED.RATE=<n>] [100.OEDF=<n>] [110.OEDF=<n>] [111.OEDF=<n>] [AFFINITY=<n>] [EPSILONF=<n>] [N.VALENC=<n>] [N.CONDUC=<n>] [BAND.GAP=<n>] [K.M=<n>]

Name	Type	Description	Unit	Default
ABUND.1	Num	The relative abundance of element one in the material. The sum of all abundances for a material must equal one.		the current value
AFFINITY	Num	The electron affinity of the material.	eV	the current value
AT.NUM.1	Num	The atomic number of element one in the material.		the current value
AT.WT.1	Num	The atomic weight of element one in the material.	amu	the current value
BAND.GAP	Num	The band gap of the material.	eV	the current value
DEFECTLN	Num	The decay length of point defects in the material.	microns	the current value
DENSITY	Num	The density of the material.	grams/cm^3	the current value
DX.DEFAU	Num	The default nominal grid spacing for any layer containing this material.	microns	the current value
EPSILONF	Num	The dielectric constant of the material relative the dielectric constant of air.		the current value
K.M	Num	Used in R. Reif's epitaxial growth model (see reference	micron	the current value

		in EPITAXY statement). K.m is the mass transport coefficient for silane in hydrogen.	s/min/atm	
NAME	Char	The name of the material.		the current name of the material
NI.0	Num	The pre-factor used in the calculation of the intrinsic carrier concentration.	(carriers/cm^3)°K$^{3/2}$	the current value
NI.E	Num	The activation energy used in the calculation of the intrinsic carrier concentration.	eV	the current value
NI.F	Num	The exponent to the absolute temperature used in the calculation of the intrinsic carrier concentration.		the current value
N.CONDUC	Num	The carrier concentration in the conduction band of the material.	carriers/cm^3	the current value
N.VALENC	Num	The carrier concentration in the valence band of the material.	carriers/cm^3	the current value
OEDK.0	Num	The pre-exponential constant used to calculate the relative contribution of oxidation enhanced diffusion to intrinsic diffusion.		the current value
OEDK.E	Num	The activation energy used to calculate the relative contribution of oxidation enhanced diffusion to intrinsic diffusion.	eV	the current value
OED.RATE	Num	The power dependence of oxidation enhanced diffusion on the oxidation rate.		the current value
SEMICOND	Log	Specifies that the material is a semiconductor.		false
SPECIES	Num	The number of different elements in this material.		the current value
100.OEDF	Num	The orientation dependent factor for oxidation enhanced diffusion for <100> oriented silicon.		the current value
110.OEDF	Num	The orientation dependent factor for oxidation enhanced diffusion for <110> oriented silicon.		the current value
111.OEDF	Num	The orientation dependent factor for oxidation enhanced diffusion for <111> oriented silicon.		the current value

The SILICON statement is an alias for the MATERIAL statement with an index of one and is used to define or modify the parameters and coefficients associated with the material silicon. Not all of the parameters of the MATERIAL statement apply to silicon and so are not listed here.

XXXVIII.Solubility Statement

The SOLUBILITY statement is used to input a table of ordered temperature/solubility pairs. This data is used by the program to calculate the solid solubility of the various impurities in the materials present in the structure.

SOLUBILITY
FILE=<c> CONC.COL=<n> TEMP.COL=<n> [SKIP=<n>] [COUNT=<n>] [COM.CHAR=<c>] (ANTIMONY | ARSENIC | BORON | PHOSPHOR) (ALUMINUM | NITRIDE | OXIDE | POLYSILICON | SILICON)

Name	Type	Description	Default	Synonym
ALUMINUM	Log	Specifies that the solubility data applies to the impurity in the material aluminum.	false	
ANTIMONY	Log	Specifies that the solubility data applies to the dopant	false	SB

		antimony.		
ARSENIC	Log	Specifies that the solubility data applies to the dopant arsenic.	false	AS
BORON	Log	Specifies that the solubility data applies to the dopant boron.	false	
COM.CHAR	Char	Specifies the comment character for the lines in the file. Any line with this character in column one is ignored.	*	
CONC.COL	Num	Specifies the column in the data file containing the solubility associated with the corresponding temperature value.		
COUNT	Num	Specifies the number of data points to be input.	Input all every data point	
NITRIDE	Log	Specifies that the solubility data applies to the impurity in the material nitride.	false	
OXIDE	Log	Specifies that the solubility data applies to the impurity in the material oxide.	false	
PHOSPHOR	Log	Specifies that the solubility data applies to the dopant phosphorus.	false	
POLYSILI	Log	Specifies that the solubility data applies to the impurity in the material polysilicon.	false	
SKIP	Num	Specifies the number of data points to be skipped on input.	0	
SILICON	Log	Specifies that the solubility data applies to the impurity in the material silicon.	false	
TEMP.COL	Num	Specifies the column in the data file containing the temperature associated with the corresponding solubility values.		

The SOLUBILITY statement inputs the solubility vs. temperature data from the specified file and associates it with one or more impurities in one or more materials. The data files must be organized in columns, with one column containing the temperature values and another containing corresponding solubility concentrations. The data in the columns must be organized such that the temperature values are in increasing order. Comment lines may appear at any point as long as they are preceded the comment character in column one.

XXXIX.Stop Statement

The STOP statement terminates the SUPREM-III execution.

STOP [<c>]

The STOP statement is usually the last statement in the input stream. Any statements following an STOP statement are ignored by the program. The optional character string on the STOP statement is ignored by the program and is used for input documentation purposes only.

XL. Title Statement

The TITLE statement is used to input a character string to label the following input sequence.

TITLE [<c>]

The character string associated with the TITLE statement is output to the standard output device. If the previous statement was not either another TITLE statement nor a COMMENT statement, then a top-of-form is issued before the character string is output.

XLI. Vol.Ratio Statement

The VOL.RATIO statement is used to set the volume ratio between two materials, where one material might be converted into the material as in silicon to silicon dioxide.

VOL.RATIO
(SILICON | OXIDE | POLYSILI | NITRIDE | ALUMINUM) (/SILICON | /OXIDE | /POLYSIL | /NITRIDE | /ALUMINUM) RATIO=<n>

Name	Type	Description	Default	Synonym
ALUMINUM	Num	Specifies that the constant is the volume ratio of aluminum to the other material specified.	false	
NITRIDE	Log	Specifies that the constant is the volume ratio of silicon nitride to the other material specified.	false	
OXIDE	Log	Specifies that the constant is the volume ratio of silicon dioxide to the other material specified.	false	
POLYSILI	Log	Specifies that the constant is the volume ratio of polycrystalline silicon to the other material specified.	false	
RATIO	Num	The volume ratio between the materials specified.	the current value	CONSTANT
SILICON	Log	Specifies that the constant is the volume ratio of silicon to the other material specified.	false	
/ALUMINU	Log	Specifies that the constant is the volume ratio of the other material specified to aluminum.	false	
/NITRIDE	Log	Specifies that the constant is the volume ratio of the other material specified to silicon nitride.	false	
/OXIDE	Log	Specifies that the constant is the volume ratio of the other material specified to silicon dioxide.	false	
/POLYSIL	Log	Specifies that the constant is the volume ratio of the other material specified to polycrystalline silicon.	false	
/SILICON	Log	Specifies that the constant is the volume ratio of the other material specified to silicon.	false	

When oxidizing silicon, whether single crystal, poly crystalline, or silicon nitride, the oxide formed may have a different volume from that of the original material. The ratio between the volume of the original material and the resulting oxide is needed for modeling the moving interface during oxidation.

The ratio between any of the materials defined in the program can be specified, but only those between the various silicon forms and silicon dioxide are used by the program.

XLII. V.Threshold Statement

The V.THRESHOLD statement is used to calculate and print out the threshold voltage as a function of substrate bias for the current structure.

V.THRESHOLD

[V.SUB.1=<n>] [V.SUB.2=<n>] [DV.SUB=<n>] [(SURFACE | BACKSIDE | (BULKCONC=<n> (PTYPE | NTYPE)))] [Q.F=<n>] [TEMPERAT=<n>] [FILENAME=<c> [APPEND]]

Name	Type	Description	Unit	Default	Synonym
APPEND	Log	Specifies that the threshold voltage data is to be appended to the specified file. Otherwise the data will appear at the beginning of the file, deleting the previous contents of the file, if any.	False		
BACKSIDE	Log	Specifies that the substrate bias contact is at the backside of the wafer. This causes the concentration at the last or bottommost point in the current structure to be used as the concentration at the point of contact.	true		
BULKCONC	Num	Specifies the net active impurity concentration at the substrate bias contact.	atoms/cm^3		
DV.SUB	Num	The incremental substrate bias voltage. The threshold and punchthrough calculations will be done at sub-strate bias voltages from V.SUB1 to V.SUB2 in DV.SUB steps. At most 20 steps will be attempted.	V	0.5	
FILENAME	Char	Specifies the name of a file in which the calculated threshold and punchthrough voltages as a function of substrate bias are to be output. If no file is specified the data is output to the standard output.			
NTYPE	Log	Specifies that the majority impurity type at the bulk contact is n-type. Used only in conjunction with the BULKCONC parameter.		false	N-TYPE
PTYPE	Log	Specifies that the majority impurity type at the bulk contact is p-type. Used only in conjunction with the BULKCONC parameter.		false	P-TYPE
Q.F	Num	Specifies the fixed oxide charge density.	charges/ unit area	0.0	Q.SS
SURFACE	Log	Specifies that the substrate bias contact is at the top surface of the wafer. This causes the concentration at the first or topmost point in the current structure to be used as the concentration at the point of contact.		true	
TEMPERAT	Num	The calculations are done assuming that the device is operating at the temperature specified.	°C	27.0	
V.SUB1	Num	The initial substrate bias voltage used in calculating the threshold and punchthrough voltages. The threshold and punchthrough calculations will be done at substrate bias voltages from V.SUB1 to V.SUB2 in DV.SUB steps. At most 20 steps will be attempted.	V	0.0	
V.SUB2	Num	The final substrate bias voltage used in calculating the threshold and punchthrough voltages. The threshold and punchthrough calculations will be done at substrate bias voltages from V.SUB1 to V.SUB2 in DV.SUB steps. At most 20 steps will	V	5.0	

be attempted.

The V.THRESHOLD statement calculates the threshold and punchthrough voltages for the current structure at one or more substrate biases. A MIS structure must exist for the calculations to be performed. If more than one substrate bias point is desired, then the first and last and optionally the increment bias voltages are specified. The oxide fixed charge density and the substrate bias contact point may also be specified.

Normally the results of the V.THRESHOLD calculations are output to the standard output, however if a file is specified, the results are instead sent to that file. The results of several V.THRESHOLD calculations may be sent to the same file if the APPEND parameter is used.

An explanation of the algorithm used by the V.THRESHOLD statement can be found in `Calculation of Threshold Voltage in Nonuniformly Doped MOSFETS', by D. A. Antoniadis, IEEE Trans. E. D., Vol. ED-31, No. 3, March 1984, pp 303-307.

XLIII. WetO2 Statement

The WETO2 statement allows the user to modify the coefficients used to model the oxidation of the various materials under wet ambient oxidation conditions.

WETO2
[(<111> | <110> | <100>) [LIN.L.0=<n>] [LIN.L.E=<n>] [LIN.H.0=<n>] [LIN.H.E=<n>] [THINOX.0=<n>] [THINOX.E=<n>] [THINOX.L=<n>]]
[PAR.L.0=<n>] [PAR.L.E=<n>] [PAR.H.0=<n>] [PAR.H.E=<n>] [LIN.BREA=<n>] [PAR.BREA=<n>] [LIN.PDEP=<n>] [PAR.PDEP=<n>] [PRESSURE=<n>] [HCL%=<n>] [GAMMA.0=<n>] [GAMMA.E=<n>] [DELTA.0=<n>] [DELTA.E=<n>] [EXP.0=<n>] [EXP.E=<n>] [NIOX.0=<n>] [NIOX.E=<n>] [NIOX.F=<n>] [CL.ROW=<n> [CL.PCT=<n>] CL.COLUM=<n> [CL.TEMPE=<n>] [CL.DEP.L=<n>] [CL.DEP.P=<n>]]

Name	Type	Description	Unit	Default
CL.COLUM	Num	The column number in the table of coefficients used to calculate the chlorine dependence of the oxidation rates.		the current value
CL.DEP.L	Num	The coefficient modifying the linear oxidation rate in the presence of chlorine at the specified row and column.		the current value
CL.DEP.P	Num	The coefficient modifying the parabolic oxidation rate in the presence of chlorine at the specified row and column.		the current value
CL.PCT	Num	The percentage of chlorine for which the coefficients in the specified row are valid.	percent	the current value
CL.ROW	Num	The row number in the table of coefficients used to calculate the chlorine dependence of the oxidation rates.		the current value
CL.TEMPE	Num	The temperature for which the coefficients in the specified column are valid.	°C	the current value
DELTA.0	Num	The pre-exponential factor of the delta coefficient used in calculating the impurity concentration dependence of the parabolic oxidation rate.	cm^3/atom	the current value
DELTA.E	Num	The activation energy of the delta coefficient used in calculating the impurity concentration dependence of the parabolic oxidation rate.	eV	the current value
EXP.0	Num	The pre-exponential factor of the exponent used in calculating the impurity concentration dependence of the parabolic oxidation rate.		the current value
EXP.E	Num	The activation energy of the exponent used in calculating	eV	the current value

		the impurity concentration dependence of the parabolic oxidation rate.		
GAMMA.0	Num	The pre-exponential factor of the gamma coefficient used in calculating the impurity concentration dependence of the linear oxidation rate.		the current value
GAMMA.E	Num	The activation energy of the gamma coefficient used in calculating the impurity concentration dependence of the linear oxidation rate.	eV	the current value
HCL%	Num	The default percentage of chlorine present in the ambient.	percent	the current value
LIN.BREA	Num	The temperature at which the temperature dependence of the linear oxidation rate changes.	°C	the current value
LIN.H.0	Num	The pre-exponential constant of the linear oxidation rate for temperatures above the breakpoint set by L.BREAKP.	microns/min.	the current value
LIN.H.E	Num	The activation energy of the linear oxidation rate for temperatures above the breakpoint set by L.BREAKP.	eV	the current value
LIN.L.0	Num	The pre-exponential constant of the linear oxidation rate for temperatures below the breakpoint set by L.BREAKP.	microns/min.	the current value
LIN.L.E	Num	The activation energy of the linear oxidation rate for temperatures below the breakpoint set by L.BREAKP.	eV	the current value
LIN.PDEP	Num	The pressure dependence factor for the linear oxidation rate.		the current value
NIOX.0	Num	The pre-exponential constant used to determine the oxidation rate of silicon nitride.	microns	the current value
NIOX.E	Num	The activation energy used to determine the oxidation rate of silicon nitride.	eV	the current value
NIOX.F	Num	The exponent factor used to determine the oxidation rate of silicon nitride.		the current value
PAR.BREA	Num	The temperature at which the temperature dependence of the parabolic oxidation rate changes.	°C	the current value
PAR.H.0	Num	The pre-exponential constant of the parabolic oxidation rate for temperatures above the breakpoint set by P.BREAKP.	microns^2/min.	the current value
PAR.H.E	Num	The activation energy of the parabolic oxidation rate for temperatures above the breakpoint set by P.BREAKP.	eV	the current value
PAR.L.0	Num	The pre-exponential constant of the parabolic oxidation rate for temperatures below the breakpoint set by P.BREAKP.	microns^2/min.	the current value
PAR.L.E	Num	The activation energy of the parabolic oxidation rate for temperatures below the breakpoint set by P.BREAKP.	eV	the current value
PAR.PDEP	Num	The pressure dependence factor for the parabolic oxidation rate.		the current value
PRESSURE	Num	The default ambient pressure. (See note below.)	atm.	the current value
THINOX.0	Num	The pre-exponential constant of the thin oxide growth rate parameter.	microns/min.	the current value
THINOX.E	Num	The activation energy of the thin oxide growth rate parameter.	eV	the current value
THINOX.L	Num	The characteristic length of the thin oxide growth rate parameter.	microns	the current value
<100>	Log	Specifies that the linear growth rate and thin oxide		false

		growth rate parameters apply to <100> orientation silicon.	
<110>	Log	Specifies that the linear growth rate and thin oxide growth rate parameters apply to <110> orientation silicon.	false
<111>	Log	Specifies that the linear growth rate and thin oxide growth rate parameters apply to <111> orientation silicon.	false

The three oxidation model statements, DRYO2, WETO2, and NITROGEN, use identical parameters, differing only in the values assigned. The parameters NIOX.C, NIOX.E, and NIOX.F are used in modeling the oxidation silicon nitride while the others deal with the oxidation of single and polycrystalline silicon.

The effects of chlorine in the ambient gas on the oxidation rate of silicon are currently modeled by an empirical expression whose only variable is defined by the L.CLDEP and P.CLDEP for the linear and parabolic rates respectively. To date no convenient function is available to calculate the chlorine dependence as a function of temperature and amount of chlorine present, therefor a table of values defines the chlorine dependence factors at those temperatures and percentages for which reliable data is available. For those temperatures and chlorine percentages between the values in the table, linear interpolation is employed to calculate the value used. For temperatures or percentages outside the range of values present in the table, the values whose conditions most nearly match the current conditions are used. For example, if the current conditions are a temperature of 1175 degrees with three percent chlorine, but the highest temperature entry in the table is 1150 degrees and the nearest chlorine percentages are for two and four percent, then a value halfway between the values at 1150 degrees and two and four percent chlorine will be used.

NOTE: The effective oxidant partial pressure for pyrogenic steam reactors has been found to vary significantly from facility to facility. It is recommended that the user set the default pressure for WetO2 to a value that gives the best agreement with measured oxide thicknesses from his facility.

XLIV. Statement Summary

ALUMINUM

[NAME=<c>] [DX.DEFAU=<n>] [CONDUCTO] [SPECIES=<n>] [DENSITY=<n>] [AT.WT.1=<n>] [AT.NUM.1=<n>] [ABUND.1=<n>] [WORK.FUN=<n>] [EPSILONF=<n>]

ANTIMONY

[NAME=<c>] [DONOR] [AT.WT=<n>] [AT.NUMB=<n>] [IONFILE1=<c>] [IONFILE2=<c>]

[((SILICON [FII.0=<n>] [FII.E=<n>] [K.MF=<n>] [K.A=<n>] [K.P=<n>]) | (POLYSILI [FII.0=<n>] [FII.E=<n>] [ENTROPY=<n>] [HEAT.SEG=<n>] [Q.SITES=<n>]) | (OXIDE | NITRIDE | ALUMINUM)

[ELECT.ST=<n>] [DIX.0=<n>] [DIX.E=<n>] [DIM.0=<n>] [DIM.E=<n>] [DIMM.0=<n>] [DIMM.E=<n>]]

ARSENIC

[NAME=<c>] [DONOR] [AT.WT=<n>] [AT.NUMB=<n>] [IONFILE1=<c>] [IONFILE2=<c>]

[((SILICON [FII.0=<n>] [FII.E=<n>] [K.MF=<n>] [K.A=<n>] [K.P=<n>] [(IMPLANT | CHEMICAL) [CTN.0=<n>] [CTN.E=<n>] [CTN.F=<n>]]) | (POLYSILI [ENTROPY=<n>] [HEAT.SEG=<n>] [Q.SITES=<n>] [FII.0=<n>] [FII.E=<n>] [(IMPLANT | CHEMICAL) [CTN.0=<n>] [CTN.E=<n>] [CTN.F=<n>]]) | (OXIDE | NITRIDE | ALUMINUM)

[ELECT.ST=<n>] [DIX.0=<n>] [DIX.E=<n>] [DIM.0=<n>] [DIM.E=<n>] [DIMM.0=<n>] [DIMM.E=<n>]]

BIAS

LAYER=<n> ([V.ELECTR=<n>] [DV.ELECTR=<n>]) | (([DIFFUSIO=<n>] [V.MAJORI=<n>] [DV.MAJOR=<n>] [V.MINORI=<n>] [DV.MINOR=<n>]) | [FLOAT])

BORON

[NAME=<c>] [ACCEPTOR] [AT.WT=<n>] [AT.NUMB=<n>] [IONFILE1=<c>] [IONFILE2=<c>]

[((SILICON [FII.0=<n>] [FII.E=<n>] [K.MF=<n>] [K.A=<n>] [K.P=<n>]) | (POLYSILI [ENTROPY=<n>] [HEAT.SEG=<n>] [Q.SITES=<n>] [FII.0=<n>] [FII.E=<n>]) | (OXIDE | NITRIDE | ALUMINUM)

[ELECT.ST=<n>] [DIX.0=<n>] [DIX.E=<n>] [DIP.0=<n>] [DIP.E=<n>]]

COMMENT [<c>] or **$[<c>]**

DEPOSITION

THICKNES=<n>

(SILICON (<111> | <110> | <100>) | POLYSILI TEMPERAT=<n> [PRESSURE=<n> | GRAINSIZ=<n>] | OXIDE | NITRIDE | ALUMINUM)

[DX=<n>] [XDX=<n>] [SPACES=<n>] [MIN.DX=<n>] [CONCENTRATION=<n> (ANTIMONY | ARSENIC | BORON | PHOSPHOR)]

DIFFUSION

TIME=<n> TEMPERAT=<n> [T.RATE=<n>] [(GAS.CONC=<n> | SOLIDSOL) (ANTIMONY | ARSENIC | BORON | PHOSPHOR)] [(DRYO2 | WETO2 | NITROGEN) [

PRESSURE=<n>] [P.RATE=<n>] [HCL%=<n>]] [DTMIN=<n>] [DTMAX=<n>] [ABS.ERR=<n>] [REL.ERR=<n>]

DRYO2

[(<111> | <110> | <100>) [LIN.L.0=<n>] [LIN.L.E=<n>] [LIN.H.0=<n>] [LIN.H.E=<n>] [THINOX.0=<n>] [THINOX.E=<n>] [THINOX.L=<n>]]

[PAR.L.0=<n>] [PAR.L.E=<n>] [PAR.H.0=<n>] [PAR.H.E=<n>] [LIN.BREA=<n>] [PAR.BREA=<n>] [LIN.PDEP=<n>] [PAR.PDEP=<n>] [PRESSURE=<n>] [HCL%=<n>] [GAMMA.0=<n>] [GAMMA.E=<n>] [DELTA.0=<n>] [DELTA.E=<n>] [EXP.0=<n>] [EXP.E=<n>] [NIOX.0=<n>] [NIOX.E=<n>] [NIOX.F=<n>] [CL.ROW=<n> [CL.PCT=<n>] CL.COLUM=<n> [CL.TEMPE=<n>] [CL.DEP.L=<n>] [CL.DEP.P=<n>]]

ELECTRICAL

[STEPS=<n>] [EXTENT=<n>] [TEMPERAT=<n>] [ERROR=<n>] [MAX.ITER=<n>] [FILE.OUT=<c>]

END.ELEC [<c>]

EPITAXY

TEMPERAT=<n> TIME=<n> (GROWTH.R=<n> | PP.SILAN=<n>)

[(ANTIMONY | ARSENIC | BORON | PHOSPHOR) (CONCENTR=<n> | PP.DOPAN=<n>) [DTMIN=<n>] [DTMAX=<n>] [ABS.ERR=<n>] [REL.ERR=<n>]

ETCH

(SILICON | POLYSILI | OXIDE | NITRIDE | ALUMINUM) [(THICKNES=<n> | ALL)]

GRID

LAYER.<n> [THICKNES=<n>] [DX=<n>] [MIN.DX=<n>] [XDX=<n>] [SPACES=<n>]

IMPLANT

DOSE=<n> ENERGY=<n>

(ANTIMONY | ARSENIC | BF2 | BORON | PHOSPHOR)

(GAUSSIAN | 2-GAUSSI | PEARSON | (BOLTZMAN [MINSTEPS=<n>] [AT.WT=<n>] [AT.NUMB=<n>]))

IMPURITY

INDEX=<n> [NAME=<c>] [(DONOR | ACCEPTOR)] [AT.WT=<n>] [AT.NUMB=<n>] [IONFILE1=<c>] [IONFILE2=<c>]

[((SILICON [FII.0=<n>] [FII.E=<n>] [K.MF=<n>] [K.A=<n>] [K.P=<n>] [MISFITST=<n>] [CD=<n>] [MSF111FA=<n>] [MSF110FA=<n>] [MSF100FA=<n>] [DAMAGEST=<n>] [NE.0=<n>] [NE.E=<n>] [(IMPLANT | CHEMICAL) [CTN.0=<n>] [CTN.E=<n>] [CTN.F=<n>]]) | (POLYSILI [ENTROPY=<n>] [HEAT.SEG=<n>] [Q.SITES=<n>] [FII.0=<n>] [FII.E=<n>] [(IMPLANT | CHEMICAL) [CTN.0=<n>] [CTN.E=<n>] [CTN.F=<n>]]) | (OXIDE | NITRIDE | ALUMINUM)

[ELECT.ST=<n>] [DIX.0=<n>] [DIX.E=<n>] [DIM.0=<n>] [DIM.E=<n>] [DIMM.0=<n>] [DIMM.E=<n>] [DIP.0=<n>] [DIP.E=<n>]]

INITIALIZE

[(COEFFICI=<c> | FIRSTIME)] [STRUCTUR=<c>] [MIN.DX=<n>] [SAVESTEP] [THICKNES=<n>] [DX=<n>] [XDX=<n>] [SPACES=<n>]

[(SILICON (<111> | <110> | <100>) | POLYSILI (GRAINSIZ=<n> | (TEMPERAT=<n> [PRESSURE=<n>])) | OXIDE | NITRIDE | ALUMINUM) [CONCENTR=<n> (ANTIMONY | ARSENIC | BORON | PHOSPHOR)]]

LOADFILE

FILENAME=<c> (ALL | COEFFICI | STRUCTUR)

MATERIAL

[INDEX=<n>] [NAME=<c>] [DX.DEFAU=<n>] [(SEMICOND | CONDUCTO | INSULATO)] [SPECIES=<n>] [DENSITY=<n>] [AT.WT.1=<n>] [AT.WT.2=<n>] [AT.WT.3=<n>] [AT.NUM.1=<n>] [AT.NUM.2=<n>] [AT.NUM.3=<n>] [ABUND.1=<n>] [ABUND.2=<n>] [ABUND.3=<n>] [DIFX.0=<n>] [DIFX.E=<n>] [DIMX.0=<n>] [DIFM.E=<n>] [DIMMX.0=<n>] [DIFMM.E=<n>] [DIFP.0=<n>] [DIFP.E=<n>] [NI.0=<n>] [NI.E=<n>] [NI.F=<n>] [DEFECTLN=<n>] [OEDK.0=<n>] [OEDK.E=<n>] [OED.RATE=<n>] [100.OEDF=<n>] [110.OEDF=<n>] [111.OEDF=<n>] [GSZ.H.0=<n>] [GSZ.H.E=<n>] [GSZ.L.0=<n>] [GSZ.L.E=<n>] [MIN.GRAI=<n>] [TEMP.BRE=<n>] [RATIO.0=<n>] [RATIO.E=<n>] [GEO.FACT=<n>] [GBE.0=<n>] [GBE.E=<n>] [TAU.0=<n>] [TAU.E=<n>] [AFFINITY=<n>] [WORK.FUN=<n>] [EPSILONF=<n>] [N.VALENC=<n>] [N.CONDUC=<n>] [BAND.GAP=<n>] [K.M=<n>]

NITRIDE

[NAME=<c>] [DX.DEFAU=<n>] [INSULATO] [SPECIES=<n>] [DENSITY=<n>] [AT.WT.1=<n>] [AT.WT.2=<n>] [AT.NUM.1=<n>] [AT.NUM.2=<n>] [ABUND.1=<n>] [ABUND.2=<n>] [EPSILONF=<n>]

NITROGEN

[(<111> | <110> | <100>) [LIN.L.0=<n>] [LIN.L.E=<n>] [LIN.H.0=<n>] [LIN.H.E=<n>] [THINOX.0=<n>] [THINOX.E=<n>] [THINOX.L=<n>]]

[PAR.L.0=<n>] [PAR.L.E=<n>] [PAR.H.0=<n>] [PAR.H.E=<n>] [LIN.BREA=<n>] [PAR.BREA=<n>] [LIN.PDEP=<n>] [PAR.PDEP=<n>] [PRESSURE=<n>] [HCL%=<n>] [GAMMA.0=<n>] [GAMMA.E=<n>] [DELTA.0=<n>] [DELTA.E=<n>] [EXP.0=<n>] [EXP.E=<n>] [NIOX.0=<n>] [NIOX.E=<n>] [NIOX.F=<n>] [CL.ROW=<n> [CL.PCT=<n>] CL.COLUM=<n> [CL.TEMPE=<n>] [CL.DEP.L=<n>] [CL.DEP.P=<n>]]

OXIDE

[NAME=<c>] [DX.DEFAU=<n>] [INSULATO] [SPECIES=<n>] [DENSITY=<n>] [AT.WT.1=<n>] [AT.WT.2=<n>] [AT.NUM.1=<n>] [AT.NUM.2=<n>] [ABUND.1=<n>] [ABUND.2=<n>] [EPSILONF=<n>]

PHOSPHOR

[NAME=<c>] [DONOR] [AT.WT=<n>] [AT.NUMB=<n>] [IONFILE1=<c>] [IONFILE2=<c>]

[((SILICON [FII.0=<n>] [FII.E=<n>] [K.MF=<n>] [K.A=<n>] [K.P=<n>] [MISFITST=<n>] [CD=<n>] [MSF111FA=<n>] [MSF110FA=<n>] [MSF100FA=<n>] [DAMAGEST=<n>] [NE.0=<n>] [NE.E=<n>] [(IMPLANT | CHEMICAL) [CTN.0=<n>] [CTN.E=<n>] [CTN.F=<n>]]) | (POLYSILI [ENTROPY=<n>] [HEAT.SEG=<n>] [Q.SITES=<n>] [FII.0=<n>] [FII.E=<n>] [(IMPLANT | CHEMICAL) [CTN.0=<n>] [CTN.E=<n>] [CTN.F=<n>]]) | (OXIDE | NITRIDE | ALUMINUM)

[ELECT.ST=<n>] [DIX.0=<n>] [DIX.E=<n>] [DIM.0=<n>] [DIM.E=<n>] [DIMM.0=<n>] [DIMM.E=<n>]]

PLOT

[ACTIVE] [CHEMICAL] [TOTAL] [NET] [ANTIMONY] [ARSENIC] [BORON] [PHOSPHOR] [XMIN=<n>] [XMAX=<n>] [CMIN=<n>] [CMAX=<n>]

[((HP2648A | HP2623A) [CLEAR] [AXIS] [XPWIDTH=<n>] [YPWIDTH=<n>] [XPTS.IN=<n>] [YPTS.IN=<n>] [XOFSET=<n>] [YOFSET=<n>]] [LINETYPE=<n>] [FILENAME=<c>]) | (LP.PLOT [LINES/PA=<n>] [COLUMNS=<n>])]

POLYSILI

[NAME=<c>] [DX.DEFAU=<n>] [SEMICOND] [SPECIES=<n>] [DENSITY=<n>] [AT.WT.1=<n>] [AT.NUM.1=<n>] [ABUND.1=<n>] [DIFX.0=<n>] [DIFX.E=<n>] [DIMX.0=<n>] [DIFM.E=<n>] [DIMMX.0=<n>] [DIFMM.E=<n>] [DIFP.0=<n>] [DIFP.E=<n>] [NI.0=<n>] [NI.E=<n>] [NI.F=<n>] [DEFECTLN=<n>] [OEDK.0=<n>] [OEDK.E=<n>] [OED.RATE=<n>] [GSZ.H.0=<n>] [GSZ.H.E=<n>] [GSZ.L.0=<n>] [GSZ.L.E=<n>] [MIN.GRAI=<n>] [TEMP.BRE=<n>] [RATIO.0=<n>] [RATIO.E=<n>] [GEO.FACT=<n>] [GBE.0=<n>] [GBE.E=<n>] [TAU.0=<n>] [TAU.E=<n>] [AFFINITY=<n>] [EPSILONF=<n>] [N.VALENC=<n>] [N.CONDUC=<n>] [BAND.GAP=<n>]

PRINT

[CONCENTR [ACTIVE] [CHEMICAL] [ALL] [TOTAL] [NET] [ANTIMONY] [ARSENIC] [BORON] [PHOSPHOR] [XMIN=<n>] [XMAX=<n>]] [IMPURITY [ALL | (ANTIMONY | ARSENIC | BORON | PHOSPHOR)]]

[MATERIAL [ALL | (SILICON | POLYSILI | OXIDE | NITRIDE | ALUMINUM)]]

[LAYERS] [SEGREGAT] [OXIDATIO] [LINES/PA=<n>] [COLUMNS=<n>] [LU=<n> | FILENAME=<c>]

PROFILE

FILE=<c> CONC.COL=<n> X.COL=<n> [LAYER=<n>] [SKIP=<n>] [COUNT=<n>] [COM.CHAR=<c>] (ANTIMONY | ARSENIC | BORON | PHOSPHOR)

RESISTIVITY

FILE=<c> CONC.COL=<n> RES.COL=<n> [SKIP=<n>] [COUNT=<n>] [COM.CHAR=<c>] (ANTIMONY | ARSENIC | BORON | PHOSPHOR) (ALUMINUM | NITRIDE | OXIDE | POLYSILICON | SILICON)

SAVEFILE

FILENAME=<c> (ALL | COEFFICI | STRUCTUR | EXPORT)

SEGREGAT

((SILICON [100.FACT=<n>] [110.FACT=<n>] [111.FACT=<n>]) | OXIDE | POLYSILI | NITRIDE | ALUMINUM | AIR)

((/SILICON [100.FACT=<n>] [110.FACT=<n>] [111.FACT=<n>]) | /OXIDE | /POLYSIL | /NITRIDE | /ALUMINU | /AIR) (ANTIMONY | ARSENIC | BORON | PHOSPHOR)

[SEG.0=<n>] [SEG.E=<n>] [TRANS.0=<n>] [TRANS.E=<n>] [MUI.0=<n>] [MUI.E=<n>]

SILICON

[NAME=<c>] [DX.DEFAU=<n>] [SEMICOND] [SPECIES=<n>] [DENSITY=<n>] [AT.WT.1=<n>] [AT.NUM.1=<n>] [ABUND.1=<n>] [NI.0=<n>] [NI.E=<n>] [NI.F=<n>] [DEFECTLN=<n>] [OEDK.0=<n>] [OEDK.E=<n>] [OED.RATE=<n>] [100.OEDF=<n>] [110.OEDF=<n>] [111.OEDF=<n>] [AFFINITY=<n>] [EPSILONF=<n>] [N.VALENC=<n>] [N.CONDUC=<n>] [BAND.GAP=<n>] [K.M=<n>]

SOLUBILITY

FILE=<c> CONC.COL=<n> TEMP.COL=<n> [SKIP=<n>] [COUNT=<n>] [COM.CHAR=<c>] (ANTIMONY | ARSENIC | BORON | PHOSPHOR) (ALUMINUM | NITRIDE | OXIDE | POLYSILICON | SILICON)

STOP [<c>]

TITLE [<c>]

VOL.RATIO

(SILICON | OXIDE | POLYSILI | NITRIDE | ALUMINUM) (/SILICON | /OXIDE | /POLYSIL | /NITRIDE | /ALUMINUM) RATIO=<n>

V.THRESHOLD

[V.SUB.1=<n>] [V.SUB.2=<n>] [DV.SUB=<n>] [(SURFACE | BACKSIDE | (BULKCONC=<n> (PTYPE | NTYPE)))] [Q.F=<n>] [TEMPERAT=<n>] [FILENAME=<c> [APPEND]]

WETO2

[(<111> | <110> | <100>) [LIN.L.0=<n>] [LIN.L.E=<n>] [LIN.H.0=<n>] [LIN.H.E=<n>] [THINOX.0=<n>] [THINOX.E=<n>] [THINOX.L=<n>]]

[PAR.L.0=<n>] [PAR.L.E=<n>] [PAR.H.0=<n>] [PAR.H.E=<n>] [LIN.BREA=<n>] [PAR.BREA=<n>] [LIN.PDEP=<n>] [PAR.PDEP=<n>] [PRESSURE=<n>] [HCL%=<n>] [GAMMA.0=<n>] [GAMMA.E=<n>] [DELTA.0=<n>] [DELTA.E=<n>] [EXP.0=<n>] [EXP.E=<n>] [NIOX.0=<n>] [NIOX.E=<n>] [NIOX.F=<n>] [CL.ROW=<n> [CL.PCT=<n>]CL.COLUM=<n> [CL.TEMPE=<n>] [CL.DEP.L=<n>] [CL.DEP.P=<n>]]

XLV. Example 1: NMOS Silicon Gate.

Presented here is an example of the simulation of a NMOS silicon gate process. Three vertical cross-sections are simulated, one through the center of the gate region, the second through the source or drain region, and the third through the isolation or field region.

The structure was simulated using six input files. The first file simulates the processing in the active region of the device, up to the point where the process diverges for the gate and the source/drain regions. The second and third files start with the result of this first file and complete the processing for the gate region and the source/drain region respectively. The fourth file performs an electrical parameter calculation on the resulting gate region. The fifth file is similar to the first one, except that the processing effecting the field region of the device is simulated. The sixth file completes the field region processing.

The processing sequence used is listed below.

1. The process begins with a high resistivity, <100>, p-type substrate.
2. A 400 Angstrom pad layer of silicon dioxide is grown.
3. An 800 Angstrom layer of silicon nitride is deposited on top of the silicon dioxide.
4. The nitride is stripped from the areas outside of the active regions.
5. Boron is ion-implanted to increase the p doping at the surface in the field regions.
6. The field regions are then oxidized for three hours at 1000 degrees centigrade in a wet oxygen ambient.
7. Etch to the silicon surface in the active regions.
8. Ion implant boron to set the threshold voltage of the device.
9. Grow the 400 Angstrom gate oxide.
10. Deposit a half micron layer of polysilicon.
11. Dope it with phosphorus using POCl3 in a predeposition furnace.
12. Etch the polysilicon from the areas outside of the gate regions.
13. Ion implant arsenic to form the source and gate regions.
14. Drive-in the source and drain diffusions for 30 minutes at 1000 degrees centigrade in a dry oxygen ambient.
15. Open the contact holes in the gate, source, and drain regions.
16. Use CVD to deposit phosphorus doped silicon dioxide over the wafer surface.
17. Reflow the glass at 1000 degrees for 30 minutes.
18. Reopen the contact holes and deposit aluminum.

Cross-section of locally oxidized NMOS device simulated in this example.

Simulations through both the active (channel) region and through the field oxide region are shown. In addition, a Poisson solution through the channel region is used to extract threshold voltage.

```
 ********************************
 *** Suprem-III  ***
 ***version 1B  rev. 8520***
 ********************************

Fri Oct  4 21:05:05 1985

 Commands input from file: s3ex1a.in

1... Title SUPREM-III Example 1.  NMOS Silicon Gate
2... CommentActive device region initial processing.
3... $ File S3EX1A
4... CommentInitialize silicon substrate.
5... Initialize <100> Silicon, Boron Concentration=1e15
 ...+Thickness=1.5 dX=.005 XdX=.02  Spaces=150
6... CommentGrow pad oxide, 400A.
7... Diffusion  Temperature=1000  Time=40  DryO2
8... CommentDeposit 800A of CVD Nitride.
9... DepositNitride  Thickness=.0800  Spaces=15
10... CommentGrow field oxide.
11... Diffusion  Temperature=1000  Time=180  WetO2
12... Print Layer
13... CommentEtch to silicon surface.
14... Etch  Oxide all
15... Etch  Nitride all
16... Etch  Oxide all
17... CommentImplant boron to shift the threshold voltage.
18... ImplantBoron  Dose=4e11  Energy=50
19... CommentGrow gate oxide
20... Diffusion  Temperature=1050  Time=30  DryO2  HCL%=3
21... CommentDeposit polysilicon
22... DepositPolysilicon  Thickness=0.5  Temperature=600
23... CommentHeavily dope the polysilicon using POCl3
24... Diffusion  Temperature=1000  Time=25  dTmin=.3
 ...+Phosphorus  Solidsolubility
25... Print Layer
26... Plot  Chemical BoronXmax=1.5Clear ^Axis Linetype=2
27... Plot  Chemical Phosphorus  Xmax=1.5  ^Clear ^Axis Linetype=3
28... Plot  Chemical Net Xmax=1.5  ^Clear  Axis
29... CommentSave the structure at this point.  The simulation runs
30... $ are split for the gate and source/drain regions.
31... Save  Structure  File=s3e1as
32... Stop  End of SUPREM-III Example 1.
```

SUPREM-III Example 1. NMOS Silicon Gate

```
 Active device region initial processing.
 File S3EX1A
 Initialize silicon substrate.
 Grow pad oxide, 400A.
 Deposit 800A of CVD Nitride.
 Grow field oxide.
```

layer no.	material type	thickness (microns)	dx (microns)	dxmin	top node	bottom node	orientation or grain size
4	OXIDE	0.0176	0.0100	0.0010	330	332	
3	NITRIDE	0.0694	0.0100	0.0010	333	347	
2	OXIDE	0.0376	0.0100	0.0010	348	351	
1	SILICON	1.4835	0.0050	0.0010	352	500	<100>

Integrated Dopant

layer	Net		Total	
no.	active	chemical	active	chemical
4	0.e+00	0.e+00	0.e+00	0.e+00
3	0.e+00	-4.9183e+07	0.e+00	4.9183e+07
2	0.e+00	-7.0206e+09	0.e+00	7.0206e+09
1	-1.4205e+11	-1.4205e+11	1.4205e+11	1.4205e+11
sum	-1.4205e+11	-1.4912e+11	1.4205e+11	1.4912e+11

Integrated Dopant

layer	BORON	
no.	active	chemical
4	0.e+00	0.e+00
3	0.e+00	4.9183e+07
2	0.e+00	7.0206e+09
1	1.4205e+11	1.4205e+11
sum	1.4205e+11	1.4912e+11

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

layer no.	region no	type	junction depth (microns)	net active Qd	total chemical Qd
4	1	n	0.	0.e+00	0.e+00
3	2	n	0.	0.e+00	0.e+00
3	1	p	0.0694	0.e+00	0.e+00
2	1	p	0.	0.e+00	7.0206e+09
1	1	p	0.	1.4205e+11	1.4205e+11

Etch to silicon surface.
Implant boron to shift the threshold voltage.
Grow gate oxide
Deposit polysilicon
Heavily dope the polysilicon using POCl3

layer no.	material type	thickness (microns)	dx (microns)	dxmin	top node	bottom node	orientation or grain size
3	POLYSILICON	0.5000	0.0100	0.0010	299	349	0.6135
2	OXIDE	0.0477	0.0100	0.0010	350	355	
1	SILICON	1.4625	0.0050	0.0010	356	500	<100>

Integrated Dopant

layer	Net		Total	
no.	active	chemical	active	chemical
3	3.4861e+15	4.0061e+15	3.4861e+15	4.0061e+15
2	0.e+00	-8.5693e+10	0.e+00	8.5693e+10
1	-4.5461e+11	-4.5461e+11	4.5461e+11	4.5461e+11
sum	3.4857e+15	4.0056e+15	3.4866e+15	4.0067e+15

Integrated Dopant

layer	BORON		PHOSPHORUS	
no.	active	chemical	active	chemical

3	1.6362e+08	1.6362e+08	3.4861e+15	4.0061e+15
2	0.e+00	8.5693e+10	0.e+00	1.3296e+05
1	4.5461e+11	4.5461e+11	1.0017e-09	1.0017e-09
sum	4.5478e+11	5.4047e+11	3.4861e+15	4.0061e+15

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

layer no.	region no.	type	junction depth (microns)	net active Qd	total chemical Qd
3	1	n	0.	3.4861e+15	4.0061e+15
2	1	p	0.	0.e+00	8.5693e+10
1	1	p	0.	4.5461e+11	4.5461e+11

Save the structure at this point. The simulation runs are split for the gate and source/drain regions.
End Suprem-III

Suprem-III simulation after the channel implant, gate oxide growth, poly deposition and doping. Phosphorus diffusion from the poly gate into the gate oxide is evident.

```
***************************
***        Suprem-III        ***
***   version 1B  rev. 8520   ***
***************************
Fri Oct  4 21:08:21 1985
Commands input from file: s3ex1b.in
```

```
1... Title SUPREM-III Example 1.  NMOS Silicon Gate
2... CommentGate region.
3... $ File s3ex1b
4... CommentInitialize silicon substrate.
5... Initialize Structure=s3e1as
6... CommentImplant Arsenic for source/drain regions.
7... ImplantArsenic  Dose=5E15  Energy=150
8... CommentDrive-in Arsenic and re-oxidize source/drain regions.
9... Diffusion  Temperature=1000  Time=30  DryO2
10... CommentEtch contact holes to gate, source, and drain regions.
11... Etch  Oxide
12... CommentDeposit Phosphorus doped SiO2 using CVD.
13... DepositOxide  Thickness=.7500  Phosphorus Concentration=1.E21
14... CommentIncrease the diffusivity of phosphorus in oxide by
15... $  two orders of magnitude.
16... Phosphorus Oxide  Dix.0=4.56E7
17... CommentReflow glass to smooth surface and dope contact holes.
18... Diffusion  Temperature=1000  Time=30
19... CommentReopen contact holes.
20... Etch  Oxide
21... CommentDeposit Aluminum.
22... DepositAluminum  Thickness=1.2  Spaces=10
23... CommentPlot the chemical impurity distributions at this point.
24... Print Layer
25... Plot  Chemical BoronXmax=2.5Clear ^Axis Linetype=2
26... Plot  Chemical Arsenic Xmax=2.5  ^Clear ^Axis Linetype=3
27... Plot  Chemical Phosphorus  Xmax=2.5  ^Clear ^Axis Linetype=6
```

28... Plot Chemical Net Xmax=2.5 ^Clear Axis
29... CommentSave the structure.
30... Save Structure File=s3e1bs
31... Stop End of SUPREM-III Example 1.

SUPREM-III Example 1. NMOS Silicon Gate

Gate region.
File s3ex1b
Initialize silicon substrate.
Implant Arsenic for source/drain regions.
Drive-in Arsenic and re-oxidize source/drain regions.
Etch contact holes to gate, source, and drain regions.
Deposit Phosphorus doped SiO2 using CVD.
Increase the diffusivity of phosphorus in oxide by two orders of magnitude.
Reflow glass to smooth surface and dope contact holes.
Reopen contact holes.
Deposit Aluminum.
Plot the chemical impurity distributions at this point.

layer no.	material type	thickness (microns)	dx (microns)	dxmin	top node	bottom node	orientation or grain size
4	ALUMINUM	1.2000	0.0100	0.0010	291	301	
3	POLYSILICON	0.4681	0.0100	0.0010	302	349	0.9051
2	OXIDE	0.0477	0.0100	0.0010	350	355	
1	SILICON	1.4625	0.0050	0.0010	356	500	<100>

Integrated Dopant

layer	Net		Total	
no.	active	chemical	active	chemical
4	0.e+00	0.e+00	0.e+00	0.e+00
3	8.2667e+15	8.9390e+15	8.2667e+15	8.9390e+15
2	0.e+00	2.7347e+12	0.e+00	2.9065e+12
1	-4.5403e+11	-4.5403e+11	4.5403e+11	4.5403e+11
sum	8.2662e+15	8.9413e+15	8.2671e+15	8.9423e+15

Integrated Dopant

layer	PHOSPHORUS		ARSENIC	
no.	active	chemical	active	chemical
4	0.e+00	0.e+00	0.e+00	0.e+00
3	4.0103e+15	4.6114e+15	4.2563e+15	4.3276e+15
2	0.e+00	2.4041e+12	0.e+00	4.1647e+11
1	4.6984e+03	4.6984e+03	1.9015e-29	1.9015e-29
sum	4.0103e+15	4.6138e+15	4.2563e+15	4.3280e+15

Integrated Dopant

layer	BORON	
no.	active	chemical
4	0.e+00	0.e+00
3	5.3820e+08	5.3820e+08
2	0.e+00	8.5893e+10
1	4.5403e+11	4.5403e+11
sum	4.5457e+11	5.4046e+11

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

layer	region	type	junction depth	net	total

no.	no.		(microns)	active Qd	chemical Qd
4	1	n	0.	0.e+00	0.e+00
3	1	n	0.	8.2667e+15	8.9390e+15
2	2	n	0.	0.e+00	2.8436e+12
2	1	p	0.0358	0.e+00	2.7665e+10
1	1	p	0.	4.5403e+11	4.5403e+11

Save the structure.
End Suprem-III

Suprem-III simulation through the gate region following all processi steps.

```
***************************
***         Suprem-III          ***
***    version 1B  rev. 8520  ***
***************************
Fri Oct  4 21:10:44 1985
Commands input from file: s3ex1c.in
```

1... Title SUPREM-III Example 1. NMOS Silicon Gate
2... CommentSource/drain regions.
3... $ File s3ex1c
4... CommentInitialize silicon substrate.
5... Initialize Structure=s3e1as
6... CommentEtch polysilicon and oxide over source/drain regions.
7... Etch Polysilicon
8... Etch Oxide
9... CommentImplant Arsenic for source/drain regions.
10... ImplantArsenic Dose=5E15 Energy=150
11... CommentDrive-in Arsenic and re-oxidize source/drain regions.
12... Diffusion Temperature=1000 Time=30 DryO2
13... CommentEtch contact holes to gate, source, and drain regions.
14... Etch oxide
15... CommentDeposit Phosphorus doped SiO2 using CVD.
16... DepositOxide Thickness=.7500 Phosphorus Concentration=1e21
17... CommentIncrease the diffusivity of phosphorus in oxide by
18... $ two orders of magnitude.
19... Phosphorus Oxide Dix.0=4.56E7
20... CommentReflow glass to smooth surface and dope contact holes.
21... Diffusion Temperature=1000 Time=30
22... Print Layer
23... CommentReopen contact holes.
24... Etch Oxide
25... CommentDeposit Aluminum.
26... DepositAluminum Thickness=1.2 Spaces=10
27... CommentPlot the chemical impurity distributions at this point.
28... Print Layer
29... Plot Chemical BoronXmax=2.5Clear ^Axis Linetype=2
30... Plot Chemical Arsenic Xmax=2.5 ^Clear ^Axis Linetype=3
31... Plot Chemical Phosphorus Xmax=2.5 ^Clear ^Axis Linetype=6
32... Plot Chemical Net Xmax=2.5 ^Clear Axis
33... CommentSave the structure.

34... Save Structure File=s3e1cs
35... Stop End of SUPREM-III Example 1.

SUPREM-III Example 1. NMOS Silicon Gate

Source/drain regions.
File s3ex1c
Initialize silicon substrate.
Etch polysilicon and oxide over source/drain regions.
Implant Arsenic for source/drain regions.
Drive-in Arsenic and re-oxidize source/drain regions.
Error number 204 detected in line number 12
During this step,14 intermediate solutions resulted in
distributions with at least one negative concentration.
Etch contact holes to gate, source, and drain regions.
Deposit Phosphorus doped SiO2 using CVD.
Increase the diffusivity of phosphorus in oxide by
two orders of magnitude.
Reflow glass to smooth surface and dope contact holes.

layer no.	material type	thickness (microns)	dx (microns)	dxmin	top node	bottom node	orientation or grain size
2	OXIDE	0.7500	0.0100	0.0010	285	360	
1	SILICON	1.4367	0.0050	0.0010	361	500	<100>

Integrated Dopant

layer	Net		Total	
no.	active	chemical	active	chemical
2	0.e+00	7.3656e+16	0.e+00	7.3656e+16
1	5.2811e+15	5.5049e+15	5.2818e+15	5.5056e+15
sum	5.2811e+15	7.9161e+16	5.2818e+15	7.9161e+16

Integrated Dopant

layer	PHOSPHORUS		ARSENIC	
no.	active	chemical	active	chemical
2	0.e+00	7.3652e+16	0.e+00	3.4378e+12
1	6.6798e+14	6.7348e+14	4.6135e+15	4.8317e+15
sum	6.6798e+14	7.4326e+16	4.6135e+15	4.8352e+15

Integrated Dopant

layer	BORON	
no.	active	chemical
2	0.e+00	1.0536e+10
1	3.5397e+11	3.5397e+11
sum	3.5397e+11	3.6451e+11

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

layer no.	region no.	type	junction depth (microns)	net active Qd	total chemical Qd
2	1	n	0.	0.e+00	7.3656e+16
1	2	n	0.	5.2812e+15	5.5054e+15
1	1	p	0.5219	1.3184e+11	1.3691e+11

Deposit Aluminum.
Plot the chemical impurity distributions at this point.

layer no.	material type	thickness (microns)	dx (microns)	dxmin	top node	bottom node	orientation or grain size

2	ALUMINUM	1.2000	0.0100	0.0010	350	360	
1	SILICON	1.4367	0.0050	0.0010	361	500	<100>

Integrated Dopant

layer	Net		Total	
no.	active	chemical	active	chemical
2	0.e+00	0.e+00	0.e+00	0.e+00
1	5.2811e+15	5.5049e+15	5.2818e+15	5.5056e+15
sum	5.2811e+15	5.5049e+15	5.2818e+15	5.5056e+15

Integrated Dopant

layer	PHOSPHORUS		ARSENIC	
no.	active	chemical	active	chemical
2	0.e+00	0.e+00	0.e+00	0.e+00
1	6.6798e+14	6.7348e+14	4.6135e+15	4.8317e+15
sum	6.6798e+14	6.7348e+14	4.6135e+15	4.8317e+15

Integrated Dopant

layer	BORON	
no.	active	chemical
2	0.e+00	0.e+00
1	3.5397e+11	3.5397e+11
sum	3.5397e+11	3.5397e+11

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

layer	region	type	junction depth	net	total
no.	no.		(microns)	active Qd	chemical Qd
2	1	n	0.	0.e+00	0.e+00
1	2	n	0.	5.2812e+15	5.5054e+15
1	1	p	0.5219	1.3184e+11	1.3691e+11

Save the structure.
End Suprem-III

Suprem-III simulation through the source-drain region following all processing steps.

****
***Suprem-III ***
version 1B rev. 8520
****
Fri Oct 4 21:13:17 1985
Commands input from file: s3ex1d.in

1... Title SUPREM-III Example 1. NMOS Silicon Gate
2... CommentGate region electrical simulation.
3... $ File s3ex1d
4... CommentInitialize using gate region result.
5... Initialize Structure=s3e1bs
6... CommentSolve Poisson's equation with the gate biased from
7... $ 0. volts to 3. volts in .2 volt steps.
8... Electrical Steps=16
9... Bias Layer=3 Diffusion=1 V.Majority=0. dV.Majority=.2
10... End
11... Stop End of SUPREM-III Example 1.

SUPREM-III Example 1. NMOS Silicon Gate
Gate region electrical simulation.
File s3ex1d
Initialize using gate region result.

Solve Poisson's equation with the gate biased from
0. volts to 3. volts in .2 volt steps.

Required Iterations =6

layer	region	Electron Concentration	Electron Conductivity	Electron Resistivity
3	1	8.8615e+15	1.3998e-23	7.1437e+22
1	1	1.1931e+07	1.7363e-09	5.7595e+08

layer	region	Hole Concentration	Hole Conductivity	Hole Resistivity
3	1	0.e+00	0.e+00	0.e+00
1	1	2.4180e+11	9.1871e-09	1.0885e+08

Required Iterations =7

layer	region	Electron Concentration	Electron Conductivity	Electron Resistivity
3	1	8.8599e+15	1.3997e-23	7.1446e+22
1	1	2.0756e+09	2.9923e-07	3.3420e+06

layer	region	Hole Concentration	Hole Conductivity	Hole Resistivity
3	1	0.e+00	0.e+00	0.e+00
1	1	2.1519e+11	7.3465e-09	1.3612e+08

Required Iterations = 22

layer	region	Electron Concentration	Electron Conductivity	Electron Resistivity
3	1	8.8582e+15	1.3995e-23	7.1456e+22
1	1	4.2218e+10	6.0567e-06	1.6511e+05

layer	region	Hole Concentration	Hole Conductivity	Hole Resistivity
3	1	0.e+00	0.e+00	0.e+00
1	1	2.0160e+11	6.4701e-09	1.5456e+08

Required Iterations = 23

layer	region	Electron Concentration	Electron Conductivity	Electron Resistivity
3	1	8.8566e+15	1.3993e-23	7.1466e+22
1	1	1.1548e+11	1.6524e-05	6.0517e+04

layer	region	Hole Concentration	Hole Conductivity	Hole Resistivity
3	1	0.e+00	0.e+00	0.e+00
1	1	1.9771e+11	6.2277e-09	1.6057e+08

Required Iterations = 23

layer	region	Electron Concentration	Electron Conductivity	Electron Resistivity
3	1	8.8549e+15	1.3991e-23	7.1475e+22
1	1	1.9655e+11	2.8074e-05	3.5620e+04

layer	region	Hole Concentration	Hole Conductivity	Hole Resistivity
3	1	0.e+00	0.e+00	0.e+00
1	1	1.9593e+11	6.1176e-09	1.6346e+08

Required Iterations = 23

layer	region	Electron Concentration	Electron Conductivity	Electron Resistivity
3	1	8.8532e+15	1.3989e-23	7.1485e+22
1	1	2.8057e+11	4.0019e-05	2.4988e+04

layer	region	Hole Concentration	Hole Conductivity	Hole Resistivity
3	1	0.e+00	0.e+00	0.e+00
1	1	1.9487e+11	6.0532e-09	1.6520e+08

Required Iterations = 22

layer	region	Electron Concentration	Electron Conductivity	Electron Resistivity
3	1	8.8515e+15	1.3987e-23	7.1495e+22
1	1	3.6612e+11	5.2166e-05	1.9170e+04

layer	region	Hole Concentration	Hole Conductivity	Hole Resistivity
3	1	0.e+00	0.e+00	0.e+00
1	1	1.9416e+11	6.0096e-09	1.6640e+08

Required Iterations = 22

layer	region	Electron Concentration	Electron Conductivity	Electron Resistivity
3	1	8.8499e+15	1.3985e-23	7.1505e+22
1	1	4.5262e+11	6.4434e-05	1.5520e+04

layer	region	Hole Concentration	Hole Conductivity	Hole Resistivity
3	1	0.e+00	0.e+00	0.e+00

1	1	1.9363e+11	5.9779e-09	1.6728e+08

Required Iterations = 22

layer	region	Electron Concentration	Electron Conductivity	Electron Resistivity
3	1	8.8482e+15	1.3983e-23	7.1515e+22
1	1	5.3974e+11	7.6782e-05	1.3024e+04

layer	region	Hole Concentration	Hole Conductivity	Hole Resistivity
3	1	0.e+00	0.e+00	0.e+00
1	1	1.9324e+11	5.9542e-09	1.6795e+08

Required Iterations = 22

layer	region	Electron Concentration	Electron Conductivity	Electron Resistivity
3	1	8.8465e+15	1.3981e-23	7.1524e+22
1	1	6.2734e+11	8.9188e-05	1.1212e+04

layer	region	Hole Concentration	Hole Conductivity	Hole Resistivity
3	1	0.e+00	0.e+00	0.e+00
1	1	1.9293e+11	5.9354e-09	1.6848e+08

Required Iterations = 22

layer	region	Electron Concentration	Electron Conductivity	Electron Resistivity
3	1	8.8448e+15	1.3979e-23	7.1534e+22
1	1	7.1528e+11	1.0164e-04	9.8389e+03

layer	region	Hole Concentration	Hole Conductivity	Hole Resistivity
3	1	0.e+00	0.e+00	0.e+00
1	1	1.9268e+11	5.9203e-09	1.6891e+08

Required Iterations = 22

layer	region	Electron Concentration	Electron Conductivity	Electron Resistivity
3	1	8.8432e+15	1.3977e-23	7.1544e+22
1	1	8.0349e+11	1.1412e-04	8.7626e+03

layer	region	Hole Concentration	Hole Conductivity	Hole Resistivity
3	1	0.e+00	0.e+00	0.e+00
1	1	1.9247e+11	5.9075e-09	1.6928e+08

Required Iterations = 22

layer	region	Electron Concentration	Electron Conductivity	Electron Resistivity
3	1	8.8415e+15	1.3976e-23	7.1554e+22
1	1	8.9192e+11	1.2663e-04	7.8969e+03

layer	region	Hole Concentration	Hole Conductivity	Hole Resistivity
3	1	0.e+00	0.e+00	0.e+00
1	1	1.9229e+11	5.8967e-09	1.6959e+08

Required Iterations = 22

layer	region	Electron Concentration	Electron Conductivity	Electron Resistivity
3	1	8.8398e+15	1.3974e-23	7.1564e+22
1	1	9.8054e+11	1.3917e-04	7.1857e+03

layer	region	Hole Concentration	Hole Conductivity	Hole Resistivity
3	1	0.e+00	0.e+00	0.e+00
1	1	1.9213e+11	5.8873e-09	1.6986e+08

Required Iterations = 22

layer	region	Electron Concentration	Electron Conductivity	Electron Resistivity
3	1	8.8381e+15	1.3972e-23	7.1573e+22
1	1	1.0693e+12	1.5172e-04	6.5912e+03

layer	region	Hole Concentration	Hole Conductivity	Hole Resistivity
3	1	0.e+00	0.e+00	0.e+00
1	1	1.9201e+11	5.8794e-09	1.7008e+08

Required Iterations = 22

layer	region	Electron Concentration	Electron Conductivity	Electron Resistivity
3	1	8.8365e+15	1.3970e-23	7.1583e+22
1	1	1.1582e+12	1.6428e-04	6.0870e+03

layer	region	Hole Concentration	Hole Conductivity	Hole Resistivity
3	1	0.e+00	0.e+00	0.e+00
1	1	1.9189e+11	5.8725e-09	1.7028e+08

End Suprem-III

Plot of channel region conductivity vs. applied gate potential gener from Suprem-III Poisson solution. From such a plot, the threshold v can be easily calculated.

```
**************************
***  Suprem-III***
***version 1B  rev. 8520***
**************************

Fri Oct  4 21:14:31 1985

 Commands input from file: s3ex1e.in

1... Title SUPREM-III Example 1.  NMOS Silicon Gate
2... CommentIsolation region initial processing.
3... $ File s3ex1e
4... CommentInitialize silicon substrate.
5... Initialize <100> Silicon, Boron Concentration=1e15
 ...  +Thickness=3.0  dX=.01  Spaces=150
6... CommentGrow pad oxide, 400A.
7... Diffusion  Temperature=1000  Time=40  DryO2
8... CommentImplant boron to increase field region doping.
9... ImplantBoron  dose=1e13  energy=150
10... CommentGrow field oxide.
11... Diffusion  Temperature=1000  Time=180  WetO2
12... Print Layer
13... CommentImplant boron to shift the enhancement threshold voltage
14... ImplantBoron  Dose=4e11  Energy=50
15... CommentGrow gate oxide
16... Diffusion  Temperature=1050  Time=30  DryO2  HCL%=3
17... CommentDeposit polysilicon
18... DepositPolysilicon  Thickness=0.5  Temperature=600
19... CommentHeavily dope the polysilicon using POCl3
20... Diffusion  Temperature=1000  Time=25  dTmin=.3
 ...+Phosphorus  Solidsolubility
21... Print Layer
22... Plot  Chemical BoronClear ^Axis Linetype=2
23... Plot  Chemical Phosphorus  ^Clear ^Axis Linetype=3
24... Plot  Chemical Net ^Clear  Axis
25... CommentSave the structure at this point.
26... Save  Structure  File=s3e1es
27... Stop  End of SUPREM-III Example 1.

 SUPREM-III Example 1.  NMOS Silicon Gate
 Isolation region initial processing.
 File s3ex1e
 Initialize silicon substrate.
 Grow pad oxide, 400A.
 Implant boron to increase field region doping.
 Grow field oxide.
```

layer no.	material type	thickness (microns)	dx (microns)	dxmin	top node	bottom node	orientation or grain size
2	OXIDE	0.7610	0.0100	0.0010	348	374	
1	SILICON	2.6652	0.0100	0.0010	375	500	<100>

Integrated Dopant

layer	Net		Total	
no.	active	chemical	active	chemical
2	0.e+00	-6.1515e+12	0.e+00	6.1515e+12
1	-4.1597e+12	-4.1597e+12	4.1597e+12	4.1597e+12
sum	-4.1597e+12	-1.0311e+13	4.1597e+12	1.0311e+13

Integrated Dopant

layer	BORON	
no.	active	chemical
2	0.e+00	6.1515e+12
1	4.1597e+12	4.1597e+12
sum	4.1597e+12	1.0311e+13

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

layer	region	type	junction depth	net	total
no.	no.		(microns)	active Qd	chemical Qd
2	1	p	0.	0.e+00	6.1515e+12
1	1	p	0.	4.1597e+12	4.1597e+12

Implant boron to shift the enhancement threshold voltage.
Grow gate oxide
Deposit polysilicon
Heavily dope the polysilicon using POCl3

layer	material type	thickness	dx	dxmin	top	bottom	orientation
no.		(microns)	(microns)		node	node	or grain size
3	POLYSILICON	0.5000	0.0100	0.0010	297	347	0.6135
2	OXIDE	0.7657	0.0100	0.0010	348	374	
1	SILICON	2.6631	0.0100	0.0010	375	500	<100>

Integrated Dopant

layer	Net		Total	
no.	active	chemical	active	chemical
3	3.4861e+15	4.0061e+15	3.4861e+15	4.0061e+15
2	0.e+00	-6.6459e+12	0.e+00	6.6459e+12
1	-4.0648e+12	-4.0648e+12	4.0648e+12	4.0648e+12
sum	3.4821e+15	3.9954e+15	3.4902e+15	4.0168e+15

Integrated Dopant

layer	BORON		PHOSPHORUS	
no.	active	chemical	active	chemical
3	1.2079e+07	1.2079e+07	3.4861e+15	4.0061e+15
2	0.e+00	6.6459e+12	0.e+00	6.2621e+05
1	4.0648e+12	4.0648e+12	0.e+00	0.e+00
sum	4.0649e+12	1.0711e+13	3.4861e+15	4.0061e+15

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

layer	region	type	junction depth	net	total

no.	no.		(microns)	active Qd	chemical Qd
3	1	n	0.	3.4861e+15	4.0061e+15
2	1	p	0.	0.e+00	6.6459e+12
1	1	p	0.	4.0648e+12	4.0648e+12

Save the structure at this point.
End Suprem-III

Suprem-III simulation through the field oxide region after polysilic deposition and doping.

```
 **************************
 ***  Suprem-III***
 ***version 1B  rev. 8520***
 **************************

Fri Oct  4 21:15:57 1985

 Commands input from file: s3ex1f.in

1... Title SUPREM-III Example 1.  NMOS Silicon Gate
2... CommentFinal isolation region processing.
3... $ File s3ex1f
4... CommentInitialize silicon substrate.
5... Initialize Structure=s3e1es
6... CommentEtch polysilicon and oxide over source/drain regions.
7... Etch  Polysilicon
8... Etch  Oxide  Amount=.0700
9... CommentImplant Arsenic for source/drain regions.
10... ImplantArsenic  Dose=5E15  Energy=150
11... CommentDrive-in Arsenic and re-oxidize source/drain regions.
12... Diffusion  Temperature=1000  Time=30  DryO2
13... CommentDeposit Phosphorus doped SiO2 using CVD.
14... DepositOxide  Thickness=.7500  Phosphorus Concentration=1e21
15... CommentReflow glass to smooth surface and dope contact holes.
16... Diffusion  Temperature=1000  Time=30
17... CommentDeposit Aluminum.
18... DepositAluminum  Thickness=1.2  Spaces=10
19... CommentPlot the chemical impurity distributions at this point.
20... Print Layer
21... Plot  Chemical BoronClear ^Axis Linetype=2
22... Plot  Chemical Arsenic ^Clear ^Axis Linetype=3
23... Plot  Chemical Phosphorus  ^Clear ^Axis Linetype=6
24... Plot  Chemical Net ^Clear  Axis
25... CommentSave the structure.
26... Save  Structure  File=s3e1fs
27... Stop  End of SUPREM-III Example 1.

 SUPREM-III Example 1.  NMOS Silicon Gate
 Final isolation region processing.
 File s3ex1f
 Initialize silicon substrate.
 Etch polysilicon and oxide over source/drain regions.
 Implant Arsenic for source/drain regions.
 Drive-in Arsenic and re-oxidize source/drain regions.
 Deposit Phosphorus doped SiO2 using CVD.
 Reflow glass to smooth surface and dope contact holes.
 Deposit Aluminum.
 Plot the chemical impurity distributions at this point.

layer  material type  thickness   dx         dxmin   top    bottom   orientation
 no.                  (microns)   (microns)          node   node     or grain size
```

3	ALUMINUM	1.2000	0.0100	0.0010	218	228	
2	OXIDE	1.4489	0.0100	0.0010	229	374	
1	SILICON	2.6617	0.0100	0.0010	375	500	<100>

Integrated Dopant

layer	Net		Total	
no.	active	chemical	active	chemical
3	0.e+00	0.e+00	0.e+00	0.e+00
2	0.e+00	7.9315e+16	0.e+00	7.9328e+16
1	-3.9127e+12	-3.9127e+12	3.9127e+12	3.9127e+12
sum	-3.9127e+12	7.9311e+16	3.9127e+12	7.9332e+16

Integrated Dopant

layer	PHOSPHORUS		ARSENIC	
no.	active	chemical	active	chemical
3	0.e+00	0.e+00	0.e+00	0.e+00
2	0.e+00	7.4321e+16	0.e+00	5.0000e+15
1	0.e+00	0.e+00	0.e+00	0.e+00
sum	0.e+00	7.4321e+16	0.e+00	5.0000e+15

Integrated Dopant

layer	BORON	
no.	active	chemical
3	0.e+00	0.e+00
2	0.e+00	6.6170e+12
1	3.9127e+12	3.9127e+12
sum	3.9127e+12	1.0530e+13

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

layer no.	region no.	type	junction depth (microns)	net active Qd	total chemical Qd
3	1	n	0.	0.e+00	0.e+00
2	2	n	0.	0.e+00	7.9324e+16
2	1	p	0.9891	0.e+00	3.6946e+12
1	1	p	0.	3.9127e+12	3.9127e+12

Save the structure.
End Suprem-III

Suprem-III simulation through the field oxide region following all processing steps.

XLVI. Example 2: Bipolar Polysilicon Doped Emitter.

Presented here is an example of the simulation of a bipolar process with a polysilicon doped emitter. Two vertical cross-sections are simulated, one through the emitter region, and other through the isolation region.

The structure was simulated using five input files. The first file simulates the processing in the active region of the device up to the point of the isolation oxidation. The second file starts with the result of this first file and completes the processing in the active region. The third file performs an electrical parameter calculation on the resulting structure. As in the first example, the fourth file is similar to the first one, except that the processing in the isolation region is simulated. The fifth file completes the isolation region processing.

The processing sequence used is listed below.

1. The process begins with a high resistivity, <100>, p-type substrate.
2. Thermally oxidize the substrate, growing approximately one micron of silicon dioxide.
3. Remove the oxide layer from the areas where the buried layers are to be placed.
4. Ion implant antimony at a dose of $10^{15}/cm^2$. Drive in the buried layer for five hours at 1150 °C.
5. Etch the silicon dioxide from the surface.
6. Epitaxial growth of 1.6 microns of arsenic doped silicon.
7. Thermally grow a 400 Angstrom pad oxide.
8. Deposit 800 Angstroms of silicon nitride.
9. Etch the nitride and oxide from the isolation regions.
10. Etch the silicon halfway through the epi-layer.
11. Ion implant boron in the field regions to increase the surface p doping. Use a dose of $10^{13}/cm^2$ and an implant energy of 50 KeV.
12. Thermally oxidize the field regions to an oxide thickness equal to approximately one-half that of the epi-layer.
13. Strip the nitride layer.
14. Using a photoresist mask, implant the base region. Use boron at a dose of $10^{14}/cm^2$ and an energy of 50KeV.
15. Etch the oxide from the emitter region.
16. Deposit arsenic doped polysilicon.
17. Remove the polysilicon from the non-emitter regions.
18. Anneal to drive-in the emitter and activate the base diffusion.

Cross-section of locally oxidized bipolar structure simulated in this example.
Simulations through the active (emitter-base) region and through the field oxide are shown. In addition, a Poisson solution through the active region is used to calculate the base region sheet resistance as a function of collector-base voltage.

```
**************************
***Suprem-III  ***
***version 1B  rev. 8520***
**************************

  Fri Oct  4 21:17:02 1985

Commands input from file: s3ex2a.in

 1... TitleSuprem-III Example 2.  Bipolar Poly doped emitter.
 2... $  Initial active region formation.
 3... $  File s3ex2a
 4... Comment Initialize the silicon substrate.
 5... Initialize  <100> Silicon,  Boron  Concentration=5e14
  ... +  Thickness=5.  dX=.01  XdX=.05  Spaces=100
 6... Comment Grow masking oxide for non-active regions.
 7... DiffusionTemperature=1150  Time=100  WetO2
 8... Comment Etch the oxide over the buried layer regions.
 9... EtchOxide
10... Comment Implant and drive-in the antimony buried layer.
11... Implant Antimony  Dose=5E14  Energy=120
12... DiffusionTemperature=1150  Time=15  DryO2
13... DiffusionTemperature=1150  Time=300
14... PrintLayer
15... PlotNet Chemical  Xmax=5
16... Comment Etch off the oxide.
17... EtchOxide
18... Comment Grow 1.6 micron of arsenic doped epi.
19... Epitaxy Temperature=1050  Time=4  Growth.Rate=.4
  ...  + Arsenic Gas.Conc=5E15
20... Comment Grow a 400A pad oxide.
21... DiffusionTemperature=1060  Time=20  DryO2
22... Comment Deposit nitride to mask the field oxidation.
23... Deposit Nitride  Thickness=.08
24... Comment Plot the chemical impurity distributions at this point.
25... PrintLayer
26... PlotChemical Boron Xmax=5Clear  ^Axis  Linetype=2
27... PlotChemical ArsenicXmax=5  ^Clear  ^Axis  Linetype=4
28... PlotChemical Antimony  Xmax=5  ^Clear  ^Axis  Linetype=5
29... PlotChemical NetXmax=5  ^ClearAxis  Linetype=1
30... Comment Save the simulation structure at this point for use in
31... $  subsequent processing.
32... SavefileStructure  File=s3e2as
33... Stop

Suprem-III Example 2.  Bipolar Poly doped emitter.
Initial active region formation.
File s3ex2a
Initialize the silicon substrate.
Grow masking oxide for non-active regions.
Etch the oxide over the buried layer regions.
```

Implant and drive-in the antimony buried layer.

layer no.	material type	thickness (microns)	dx (microns)	dxmin	top node	bottom node	orientation or grain size
2	OXIDE	0.0692	0.0100	0.0010	422	424	
1	SILICON	4.5442	0.0100	0.0010	425	500	<100>

Integrated Dopant

layer	Net		Total	
no.	active	chemical	active	chemical
2	0.e+00	9.4142e+11	0.e+00	9.4788e+11
1	4.8900e+14	4.8900e+14	4.8942e+14	4.8942e+14
sum	4.8900e+14	4.8994e+14	4.8942e+14	4.9037e+14

Integrated Dopant

layer	BORON		ANTIMONY	
no.	active	chemical	active	chemical
2	0.e+00	3.2324e+09	0.e+00	9.4465e+11
1	2.1123e+11	2.1123e+11	4.8921e+14	4.8921e+14
sum	2.1123e+11	2.1446e+11	4.8921e+14	4.9015e+14

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

layer no.	region no.	type	junction depth (microns)	net active Qd	total chemical Qd
2	1	n	0.	0.e+00	9.4788e+11
1	2	n	0.	4.8909e+14	4.8931e+14
1	1	p	2.4666	9.6637e+10	1.0719e+11

Etch off the oxide.
Grow 1.6 micron of arsenic doped epi.
Grow a 400A pad oxide.
Deposit nitride to mask the field oxidation.
Plot the chemical impurity distributions at this point.

layer no.	Material type	thickness (microns)	dx (microns)	dxmin	top node	bottom node	orientation or grain size
3	NITRIDE	0.0800	0.0100	0.0010	291	299	
2	OXIDE	0.0408	0.0100	0.0010	300	302	
1	SILICON	6.1263	0.0100	0.0010	303	500	<100>

Integrated Dopant

layer	Net		Total	
no.	active	chemical	active	chemical
3	0.e+00	0.e+00	0.e+00	0.e+00
2	0.e+00	1.6043e+09	0.e+00	1.6043e+09
1	4.8681e+14	4.8681e+14	4.8724e+14	4.8724e+14
sum	4.8681e+14	4.8682e+14	4.8724e+14	4.8724e+14

Integrated Dopant

layer	ARSENIC		ANTIMONY	
no.	active	chemical	active	chemical
3	0.e+00	0.e+00	0.e+00	0.e+00
2	0.e+00	1.6043e+09	0.e+00	0.e+00
1	8.0041e+11	8.0041e+11	4.8622e+14	4.8622e+14
sum	8.0041e+11	8.0201e+11	4.8622e+14	4.8622e+14

Integrated Dopant

layer	BORON	
no.	active	chemical
3	0.e+00	0.e+00
2	0.e+00	1.2398e+00
1	2.1102e+11	2.1102e+11
sum	2.1102e+11	2.1102e+11

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

layer no.	region no.	type	junction depth (microns)	net active Qd	total chemical Qd
3	1	n	0.	0.e+00	0.e+00
2	1	n	0.	0.e+00	1.6043e+09
1	2	n	0.	4.8691e+14	4.8712e+14
1	1	p	4.0487	9.6358e+10	1.0728e+11

Save the simulation structure at this point for use in subsequent processing.
End Suprem-III

Suprem-III simulation of the active device region after drive-in of buried layer.

Suprem-III simulation of the active device region after drive-in of the buried layer, epi growth, and oxide/nitride deposition.

```
***************************
***Suprem-III***
***version 1B  rev. 8520 ***
***************************

  Fri Oct  4 21:25:42 1985

Commands input from file: s3ex2b.in

 1... TitleSuprem-III Example 2.  Bipolar Poly doped emitter.
 2... $  Final active device region formation.
 3... $  File s3ex2b
 4... Comment Start from the result of s3ex2a.
 5... Initialize  Structure=s3e2as
 6... Comment Field oxide growth.  Oxidation is masked by nitride.
 7... DiffusionTemperature=800Time=30 t.rate=10
 8... DiffusionTemperature=1000  Time=15  DryO2
 9... DiffusionTemperature=1100  Time=210 WetO2
10... DiffusionTemperature=1100  Time=15  DryO2
11... DiffusionTemperature=1100  Time=10 t.rate=-30
12... PrintLayer
13... PlotNet Chemical  Xmax=5
14... Comment Etch the oxide and nitride layers.
15... EtchOxide
16... EtchNitride
17... EtchOxide
18... Comment Move the fine grid to the surface.
19... GridLayer.1  Xdx=0.
20... Comment Implant the boron base.
21... Implant Boron  Dose=1E14  Energy=50
22... Comment Remove oxide from emitter region.
23... EtchOxide
24... Comment Deposit arsenic doped polysilicon for emitter contacts.
25... Deposit Polysilicon,  Thickness=.5  Temperature=620
...  +  Arsenic  Concentration=1e20
26... Comment Anneal to activate base and drive-in emitter.
27... DiffusionTemperature=1000  Time=20  WetO2
28... Comment Plot the electrically Active impurity distributions.
29... PrintLayer
30... PlotActive  BoronXmax=6Clear  ^Axis  Linetype=2
31... PlotActive  Arsenic Xmax=6  ^Clear  ^Axis  Linetype=4
32... PlotActive  AntimonyXmax=6  ^Clear  ^Axis  Linetype=5
33... PlotActive  Net Xmax=6  ^ClearAxis  Linetype=1

34... Comment Save the resulting active region.
35... SavefileStructure  File=s3e2bs
36... Stop

Suprem-III Example 2.  Bipolar Poly doped emitter.
Final active device region formation.
File s3ex2b
```

Start from the result of s3ex2a.

Field oxide growth. Oxidation is masked by nitride.

layer no.	material type	thickness (microns)	dx (microns)	dxmin	top node	bottom node	orientation or grain size
4	OXIDE	0.0694	0.0100	0.0010	289	294	
3	NITRIDE	0.0380	0.0100	0.0010	295	299	
2	OXIDE	0.0408	0.0100	0.0010	300	302	
1	SILICON	6.1263	0.0100	0.0010	303	500	<100>

Integrated Dopant

layer	Net		Total	
no.	active	chemical	active	chemical
4	0.e+00	0.e+00	0.e+00	0.e+00
3	0.e+00	3.8665e+06	0.e+00	3.8875e+06
2	0.e+00	1.4591e+09	0.e+00	1.5386e+09
1	4.8681e+14	4.8681e+14	4.8723e+14	4.8723e+14
sum	4.8681e+14	4.8681e+14	4.8723e+14	4.8724e+14

Integrated Dopant

layer	ARSENIC		ANTIMONY	
no.	active	chemical	active	chemical
4	0.e+00	0.e+00	0.e+00	0.e+00
3	0.e+00	3.8770e+06	0.e+00	1.1437e-01
2	0.e+00	1.4988e+09	0.e+00	6.7728e+02
1	8.0049e+11	8.0049e+11	4.8622e+14	4.8622e+14
sum	8.0049e+11	8.0199e+11	4.8622e+14	4.8622e+14

Integrated Dopant

layer	BORON	
no.	active	chemical
4	0.e+00	0.e+00
3	0.e+00	1.0495e+04
2	0.e+00	3.9734e+07
1	2.1098e+11	2.1098e+11
sum	2.1098e+11	2.1102e+11

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

layer no.	region no.	type	junction depth (microns)	net active Qd	total chemical Qd
4	1	n	0.	0.e+00	0.e+00
3	1	n	0.	0.e+00	3.8875e+06
2	1	n	0.	0.e+00	1.5386e+09
1	2	n	0.	4.8690e+14	4.8714e+14
1	1	p	4.3432	8.2905e+10	9.1476e+10

Etch the oxide and nitride layers.
Move the fine grid to the surface.
Implant the boron base.

Remove oxide from emitter region.
Error number 210 detected in line number 23
The material to be etched did not match the top material.
No etching occured.
Deposit arsenic doped polysilicon for emitter contacts.
Anneal to activate base and drive-in emitter.
Plot the electrically Active impurity distributions.

layer no.	material type	thickness (microns)	dx (microns)	dxmin	top node	bottom node	orientation or grain size
3	OXIDE	0.2922	0.0100	0.0010	250	264	
2	POLYSILICON	0.3714	0.0100	0.0010	265	302	0.5466
1	SILICON	6.1263	0.0100	0.0010	303	500	<100>

Integrated Dopant

layer	Net		Total	
no.	active	chemical	active	chemical
3	0.e+00	6.6702e+14	0.e+00	6.6703e+14
2	3.8400e+15	3.9648e+15	3.8518e+15	3.9766e+15
1	7.4183e+14	7.4352e+14	9.3043e+14	9.3212e+14
sum	4.5819e+15	5.3753e+15	4.7823e+15	5.5757e+15

Integrated Dopant

layer	ARSENIC		ANTIMONY	
no.	active	chemical	active	chemical
3	0.e+00	6.6702e+14	0.e+00	1.2424e+01
2	3.8459e+15	3.9707e+15	3.2813e+04	3.2813e+04
1	3.4991e+14	3.5160e+14	4.8622e+14	4.8622e+14
sum	4.1958e+15	4.9893e+15	4.8622e+14	4.8622e+14

Integrated Dopant

layer	BORON	
no.	active	chemical
3	0.e+00	5.3196e+09
2	5.9072e+12	5.9072e+12
1	9.4298e+13	9.4298e+13
sum	1.0021e+14	1.0021e+14

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

layer no.	region no.	type	junction depth (microns)	net active Qd	total chemical Qd
3	1	n	0.	0.e+00	6.6703e+14
2	1	n	0.	3.8400e+15	3.9766e+15
1	4	n	0.	3.2757e+14	3.5974e+14
1	3	p	0.0919	7.4602e+13	7.7270e+13
1	2	n	0.4739	4.8664e+14	4.8690e+14
1	1	p	4.3348	8.2976e+10	9.2184e+10

Save the resulting active region.

End Suprem-III

Suprem-III simulation of the active device region following field ox The Si3N4 has masked the oxidation in this region, although it has b partially oxidized itself. The Antimony buried layer has diffused u during the local oxidation process.
Suprem-III simulation of the active device region following all processing steps.
The original N epi layer has almost disappeared because of buried la base diffusion

```
*************************
***Suprem-III ***
***version 1B  rev. 8520***
*************************

  Fri Oct  4 21:32:18 1985

Commands input from file: s3ex2c.in

 1... TitleSuprem-III Example 2.  Bipolar Poly doped emitter.
 2... $  Electrical simulation of the active device region.
 3... $  File s3ex2c.

 4... Comment Start with the result of the active device region simulati
 5... Initialize  Structure=s3e2bs

 6... Comment Solve Poisson's equation with the collector ramped
 7... $  from 0 volts to 6 volts in 2 volt steps.
 8... Electrical  Extent=3  Steps=4
 9... BiasLayer=1Diffusion=3  V.Minority=0  DV.Minority=2
10... BiasLayer=1Diffusion=2  V.Majority=0  DV.Majority=2
11... BiasLayer=1Diffusion=1  V.Minority=0  DV.Minority=2
12... End

13... Stop

Suprem-III Example 2.  Bipolar Poly doped emitter.
Electrical simulation of the active device region.
File s3ex2c.
Start with the result of the active device region simulation.

Solve Poisson's equation with the collector ramped from 0 volts to 6 volts in 2 volt steps.

 Required Iterations =6
```

layer	region	Electron Concentration	Electron Conductivity	Electron Resistivity
2	1	3.9645e+15	6.2340e-24	1.6041e+23
1	4	3.2943e+14	2.7725e-02	3.6068e+01
1	3	1.4026e+02	2.3835e-15	4.1955e+14
1	2	4.8641e+14	6.0860e-03	1.6431e+02
1	1	6.0756e+06	1.1065e-09	9.0374e+08

layer	region	Hole Concentration	Hole Conductivity	Hole Resistivity
2	1	0.e+00	0.e+00	0.e+00
1	4	0.e+00	0.e+00	0.e+00
1	3	7.2010e+13	6.6469e-04	1.5045e+03
1	2	1.0366e+08	5.1626e-09	1.9370e+08
1	1	1.8942e+11	1.1792e-09	8.4804e+08

Required Iterations = 11

layer	region	Electron Concentration	Electron Conductivity	Electron Resistivity
2	1	3.9645e+15	6.2340e-24	1.6041e+23
1	4	3.2943e+14	2.7725e-02	3.6068e+01
1	3	0.e+00	0.e+00	0.e+00
1	2	4.8605e+14	6.0857e-03	1.6432e+02
1	1	0.e+00	0.e+00	0.e+00

layer	region	Hole Concentration	Hole Conductivity	Hole Resistivity
2	1	0.e+00	0.e+00	0.e+00
1	4	0.e+00	0.e+00	0.e+00
1	3	7.1722e+13	6.6436e-04	1.5052e+03
1	2	6.4678e+01	3.0993e-15	3.2265e+14
1	1	1.2595e+11	7.8543e-10	1.2732e+09

Required Iterations = 10

layer	region	Electron Concentration	Electron Conductivity	Electron Resistivity
2	1	3.9645e+15	6.2340e-24	1.6041e+23
1	4	3.2943e+14	2.7725e-02	3.6068e+01
1	3	0.e+00	0.e+00	0.e+00
1	2	4.8578e+14	6.0855e-03	1.6433e+02
1	1	0.e+00	0.e+00	0.e+00

layer	region	Hole Concentration	Hole Conductivity	Hole Resistivity
2	1	0.e+00	0.e+00	0.e+00
1	4	0.e+00	0.e+00	0.e+00
1	3	7.1485e+13	6.6396e-04	1.5061e+03
1	2	0.e+00	0.e+00	0.e+00
1	1	8.5169e+10	5.3112e-10	1.8828e+09

Required Iterations = 11

layer	region	Electron Concentration	Electron Conductivity	Electron Resistivity
2	1	3.9645e+15	6.2340e-24	1.6041e+23
1	4	3.2943e+14	2.7725e-02	3.6068e+01
1	3	0.e+00	0.e+00	0.e+00
1	2	4.8553e+14	6.0852e-03	1.6433e+02
1	1	0.e+00	0.e+00	0.e+00

layer	region	Hole Concentration	Hole Conductivity	Hole Resistivity
2	1	0.e+00	0.e+00	0.e+00
1	4	0.e+00	0.e+00	0.e+00
1	3	7.1268e+13	6.6352e-04	1.5071e+03

1	2	0.e+00	0.e+00	0.e+00
1	1	5.2488e+10	3.2732e-10	3.0551e+09

End Suprem-III

Plot of base region sheet resistance vs. collector base voltage base upon a Suprem-III Poisson solution through the active device region.

```
********************************
***Suprem-III ***
*** version 1B  rev. 8520 ***
********************************

  Fri Oct  4 21:32:58 1985

Commands input from file: s3ex2d.in

 1... TitleSuprem-III Example 2.  Bipolar Poly Doped Emitter
 2... $  Initial isolation region formation.
 3... $  File s3ex2d.
 4... Comment Initialize the silicon substrate.
 5... Initialize  <100> Silicon, Boron  Concentration=5E14
  ... +  Thickness=3  dX=.03  Spaces=75
 6... Comment Grow masking oxide for the non-active regions.
 7... DiffusionTemperature=1150  Time=100  WetO2
 8... Comment Implant and drive in the antimony buried layer.
 9... Implant Antimony  Dose=1E15  Energy=80
10... DiffusionTemperature=1150  Time=15DryO2
11... DiffusionTemperature=1150  Time=300
12... PrintLayer
13... PlotNet Chemical  Xmax=4.5
14... Comment Etch off the oxide.
15... EtchOxide
16... Comment Add 1.6 microns of arsenic doped epi.
17... Epitaxy Temperature=1050  Time=4  Growth.Rate=.4
  ... +Arsenic  Gas.Conc=5E15
18... Comment Grow a 400A pad oxide.
19... DiffusionTemperature=1060  Time=20  DryO2
20... Comment Deposit a 800A layer of silicon-nitride.
21... Deposit Nitride  Thickness=.08
22... Comment Plot the chemical impurity distributions at this point.
23... PrintLayer
24... PlotChemical  Boron Xmax=5Clear  ^Axis  Linetype=2
25... PlotChemical  ArsenicXmax=5^Clear  ^Axis  Linetype=4
26... PlotChemical  Antimony  Xmax=5^Clear  ^Axis  Linetype=5
27... PlotChemical  NetXmax=5^ClearAxis  Linetype=1
28... Comment Save the initial part of the isolation simulation.
29... SavefileStructure  File=s3e2ds
30... Stop

Suprem-III Example 2.  Bipolar Poly Doped Emitter
Initial isolation region formation.
File s3ex2d.
Initialize the silicon substrate.
Grow masking oxide for the non-active regions.
Implant and drive in the antimony buried layer.

  layer    material    thickness    dx    dxmin    top    bottom    orientation
             type
```

no.		(microns)	(microns)		node	node	or grain size
2	OXIDE	0.9752	0.0100	0.0010	423	437	
1	SILICON	2.5709	0.0300	0.0010	438	500	<100>

Integrated Dopant

layer	Net		Total	
no.	active	chemical	active	chemical
2	0.e+00	3.0849e+14	0.e+00	3.0856e+14
1	-1.1381e+11	-1.1381e+11	1.1381e+11	1.1381e+11
sum	-1.1381e+11	3.0837e+14	1.1381e+11	3.0867e+14

Integrated Dopant

layer	BORON		ANTIMONY	
no.	active	chemical	active	chemical
2	0.e+00	3.5231e+10	0.e+00	3.0852e+14
1	1.1381e+11	1.1381e+11	0.e+00	0.e+00
sum	1.1381e+11	1.4904e+11	0.e+00	3.0852e+14

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

layer	region	type	junction depth	net	total
no.	no.		(microns)	active Qd	chemical Qd
2	2	n	0.	0.e+00	3.0851e+14
2	1	p	0.5048	0.e+00	1.9102e+10
1	1	p	0.	1.1381e+11	1.1381e+11

Etch off the oxide.
Add 1.6 microns of arsenic doped epi.
Grow a 400A pad oxide.
Deposit a 800A layer of silicon-nitride.

Plot the chemical impurity distributions at this point.

layer	material type	thickness	dx	dxmin	top	bottom	orientation
no.		(microns)	(microns)		node	node	or grain size
3	NITRIDE	0.0800	0.0100	0.0010	382	390	
2	OXIDE	0.0410	0.0100	0.0010	391	393	
1	SILICON	4.1529	0.0300	0.0010	394	500	<100>

Integrated Dopant

layer	Net		Total	
no.	active	chemical	active	chemical
3	0.e+00	0.e+00	0.e+00	0.e+00
2	0.e+00	1.8392e+09	0.e+00	1.8392e+09
1	6.8788e+11	6.8788e+11	9.1491e+11	9.1491e+11
sum	6.8788e+11	6.8972e+11	9.1491e+11	9.1675e+11

Integrated Dopant

layer	BORON		ARSENIC	
no.	active	chemical	active	chemical
3	0.e+00	0.e+00	0.e+00	0.e+00
2	0.e+00	2.2662e+00	0.e+00	1.8392e+09

1	1.1351e+11	1.1351e+11	8.0140e+11	8.0140e+11
sum	1.1351e+11	1.1351e+11	8.0140e+11	8.0324e+11

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

layer no.	region no.	type	junction depth (microns)	net active Qd	total chemical Qd
3	1	n	0.	0.e+00	0.e+00
2	1	n	0.	0.e+00	1.8392e+09
1	2	n	0.	7.9326e+11	8.0645e+11
1	1	p	1.7288	1.0531e+11	1.0634e+11

Save the initial part of the isolation simulation.
End Suprem-III

Suprem-III simulation of the field oxide isolation region after driv the buried layer.
Suprem-III simulation of the field oxide isolation region after epi and oxide/nitride deposition.

```
************************* **
***  Suprem-III  ***
***version 1B  rev. 8520***
***************************

  Fri Oct  4 21:35:35 1985

Commands input from file: s3ex2e.in

 1... TitleSuprem-III Example 2.  Bipolar Poly doped emitter.
 2... $  Final isolation region formation.
 3... $  File s3ex2e.
 4... Comment Start with the result of S3EX2D.
 5... Initialize  Structure=s3e2ds  Thickness=6
 6... Comment Etch the nitride and oxide layers.
 7... EtchNitride
 8... EtchOxide
 9... Comment Etch half the silicon epi layer.
10... EtchSilicon  Amount=.8
11... Comment Implant boron in the field region.
12... Implant Boron  Dose=2E13  Energy=100
13... Comment Grow the field oxide.
14... DiffusionTemperature=800Time=30 T.Rate=10
15... DiffusionTemperature=1100  Time=15DryO2
16... DiffusionTemperature=1100  Time=210  WetO2
17... DiffusionTemperature=1100  Time=15DryO2
18... DiffusionTemperature=1100  Time=10 T.Rate=-30
19... PrintLayer
20... Comment Implant the boron base.
21... Implant Boron  Dose=1E14  Energy=80
22... Comment Deposit arsenic doped polysilicon for the emitter contact.
23... Deposit Polysilicon,  Thickness=.5  Temperature=620.
  ...+ Arsenic  Concentration=1E20
24... Comment Remove the polysilicon.
25... EtchPolysilicon
26... Comment Anneal to activate base and emitter regions.
27... DiffusionTemperature=1000  Time=20  WetO2
28... Comment Plot the electrically active impurity distributions.
29... PrintLayer
30... PlotActive  BoronXmax=5Clear  ^Axis  Linetype=2
31... PlotActive  Arsenic Xmax=5^Clear  ^Axis  Linetype=4
32... PlotActive  AntimonyXmax=5^Clear  ^Axis  Linetype=5
33... PlotActive  Net Xmax=5^ClearAxis  Linetype=1
34... Comment Save the final isolation region simulation.
35... SavefileStructure  File=s3e2es
36... Stop

Suprem-III Example 2.  Bipolar Poly doped emitter.
Final isolation region formation.
File s3ex2e.
Start with the result of S3EX2D.
```

Etch the nitride and oxide layers.
Etch half the silicon epi layer.
Implant boron in the field region.
Grow the field oxide.

layer no.	material type	thickness (microns)	dx (microns)	dxmin	top node	bottom node	orientation or grain size
2	OXIDE	1.2357	0.0100	0.0010	412	427	
1	SILICON	4.6563	0.0300	0.0010	428	500	<100>

Integrated Dopant

layer	Net		Total	
no.	active	chemical	active	chemical
2	0.e+00	-1.3771e+13	0.e+00	1.4035e+13
1	-4.9493e+12	-4.9493e+12	5.4422e+12	5.4422e+12
sum	-4.9493e+12	-1.8720e+13	5.4422e+12	1.9478e+13

Integrated Dopant

layer	BORON		ARSENIC	
no.	active	chemical	active	chemical
2	0.e+00	1.3903e+13	0.e+00	1.3241e+11
1	5.1957e+12	5.1957e+12	2.4646e+11	2.4646e+11
sum	5.1957e+12	1.9099e+13	2.4646e+11	3.7886e+11

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

layer no.	region no.	type	junction depth (microns)	net active Qd	total chemical Qd
2	1	p	0.	0.e+00	1.4035e+13
1	2	n	0.	1.5444e+10	5.6460e+10
1	1	p	0.0452	4.9231e+12	5.3460e+12

Implant the boron base.
Deposit arsenic doped polysilicon for the emitter contact.
Remove the polysilicon.
Anneal to activate base and emitter regions.
Plot the electrically active impurity distributions.

Layer no.	material type	thickness	dx (microns)	dxmin (microns)	top node	bottom node	orientation or grain size
2	OXIDE	1.2689	0.0100	0.0010	412	427	
1	SILICON	4.6417	0.0300	0.0010	428	500	<100>

Integrated Dopant

layer	Net		Total	
no.	active	chemical	active	chemical
2	0.e+00	-1.1433e+14	0.e+00	1.1460e+14
1	-4.8363e+12	-4.8363e+12	5.3259e+12	5.3259e+12
sum	-4.8363e+12	-1.1917e+14	5.3259e+12	1.1993e+14

Integrated Dopant

layer	BORON		ARSENIC	
no.	active	chemical	active	chemical
2	0.e+00	1.1447e+14	0.e+00	1.3411e+11
1	5.0811e+12	5.0811e+12	2.4476e+11	2.4476e+11

sum	5.0811e+12	1.1955e+14	2.4476e+11	3.7886e+11

Junction Depths and Integrated Dopant
Concentrations for Each Diffused Region

layer no.	region no.	type	junction depth (microns)	net active Qd	total chemical Qd
2	1	p	0.	0.e+00	1.1460e+14
1	1	p	0.	4.8363e+12	5.3259e+12

Save the final isolation region simulation.
End Suprem-III

Suprem-III simulation through the field oxide isolation region after processing steps. Isolation has been achieved since the substrate i p type, although barely. The base implant is also seen in the field

XLVII.Suggestions and Bug Reports

In any program of the size of Suprem-III there is bound to be at least one bug (Do I hear some laughter?). And even if everything works as claimed, there will always be room for improvement. There fore, I am listing both an electronic and U.S. mail address for such things as bug reports, suggestions, complaints, and compliments (if any).

Please send as much detail as possible about the problem and especially indicate which version of the program you are using and what system you are working on.

Electronic MailU.S Mail

sup3bugs@SU-FujiSuprem-III
c/o Stephen E. Hansen
Applied Electronics Labs
Stanford University
Stanford, California
94305

If you can manage it I really prefer electronic mail as it makes response easier. In either case the response time will depend on a number of factors, primarily the severity of the problem.

Your feedback is critical and appreciated!

Thanks,

Stephen E. Hansen